



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:32 pm BST

PDB ID : 4V0U
Title : The crystal structure of ternary PP1G-PPP1R15B and G-actin complex
Authors : Chen, R.; Yan, Y.; Casado, A.C.; Ron, D.; Read, R.J.
Deposited on : 2014-09-18
Resolution : 7.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

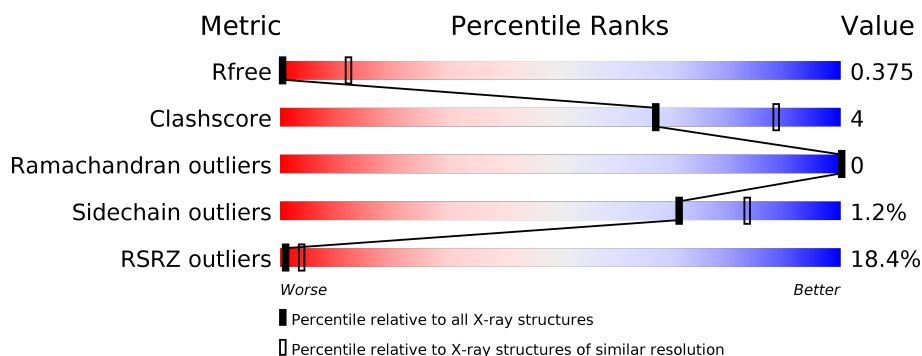
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	
1	C	375	
1	L	375	
1	M	375	
2	D	323	

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Mol	Chain	Length	Quality of chain
2	F	323	
2	H	323	
2	J	323	
2	N	323	
3	E	84	
3	G	84	
3	I	84	
3	K	84	
3	O	84	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LAB	B	1376	-	-	-	X
4	LAB	C	1376	-	-	-	X
5	ATP	L	1377	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27065 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	B	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	C	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	L	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			
1	M	364	Total	C	N	O	S	0	0	0
			2835	1796	476	544	19			

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	F	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	H	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	J	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			
2	N	294	Total	C	N	O	S	0	0	0
			2351	1509	393	432	17			

- Molecule 3 is a protein called PROTEIN PHOSPHATASE 1 REGULATORY SUBUNIT 15B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	0	0	0
			167	107	25	35			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	20	Total 167	C 107	N 25	O 35	0	0	0
3	I	20	Total 167	C 107	N 25	O 35	0	0	0
3	K	20	Total 167	C 107	N 25	O 35	0	0	0
3	O	20	Total 167	C 107	N 25	O 35	0	0	0

There are 65 discrepancies between the modelled and reference sequences:

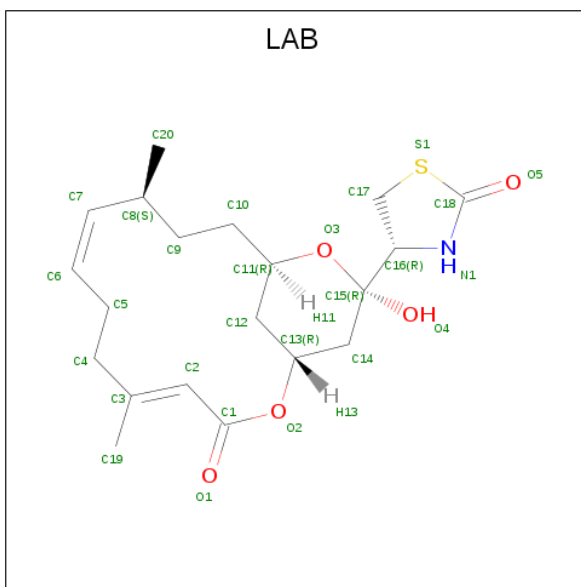
Chain	Residue	Modelled	Actual	Comment	Reference
E	626	GLY	-	expression tag	UNP Q5SWA1
E	627	ALA	-	expression tag	UNP Q5SWA1
E	628	MET	-	expression tag	UNP Q5SWA1
E	629	ASP	-	expression tag	UNP Q5SWA1
E	630	PRO	-	expression tag	UNP Q5SWA1
E	702	LEU	-	expression tag	UNP Q5SWA1
E	703	GLU	-	expression tag	UNP Q5SWA1
E	704	HIS	-	expression tag	UNP Q5SWA1
E	705	HIS	-	expression tag	UNP Q5SWA1
E	706	HIS	-	expression tag	UNP Q5SWA1
E	707	HIS	-	expression tag	UNP Q5SWA1
E	708	HIS	-	expression tag	UNP Q5SWA1
E	709	HIS	-	expression tag	UNP Q5SWA1
G	626	GLY	-	expression tag	UNP Q5SWA1
G	627	ALA	-	expression tag	UNP Q5SWA1
G	628	MET	-	expression tag	UNP Q5SWA1
G	629	ASP	-	expression tag	UNP Q5SWA1
G	630	PRO	-	expression tag	UNP Q5SWA1
G	702	LEU	-	expression tag	UNP Q5SWA1
G	703	GLU	-	expression tag	UNP Q5SWA1
G	704	HIS	-	expression tag	UNP Q5SWA1
G	705	HIS	-	expression tag	UNP Q5SWA1
G	706	HIS	-	expression tag	UNP Q5SWA1
G	707	HIS	-	expression tag	UNP Q5SWA1
G	708	HIS	-	expression tag	UNP Q5SWA1
G	709	HIS	-	expression tag	UNP Q5SWA1
I	626	GLY	-	expression tag	UNP Q5SWA1
I	627	ALA	-	expression tag	UNP Q5SWA1
I	628	MET	-	expression tag	UNP Q5SWA1
I	629	ASP	-	expression tag	UNP Q5SWA1
I	630	PRO	-	expression tag	UNP Q5SWA1

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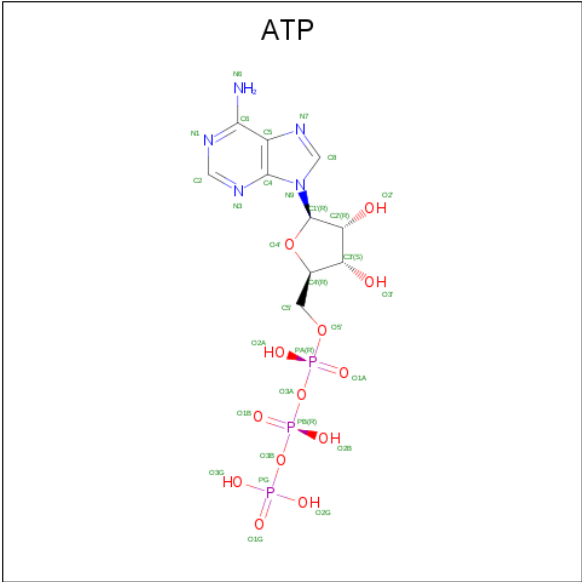
Chain	Residue	Modelled	Actual	Comment	Reference
I	702	LEU	-	expression tag	UNP Q5SWA1
I	703	GLU	-	expression tag	UNP Q5SWA1
I	704	HIS	-	expression tag	UNP Q5SWA1
I	705	HIS	-	expression tag	UNP Q5SWA1
I	706	HIS	-	expression tag	UNP Q5SWA1
I	707	HIS	-	expression tag	UNP Q5SWA1
I	708	HIS	-	expression tag	UNP Q5SWA1
I	709	HIS	-	expression tag	UNP Q5SWA1
K	626	GLY	-	expression tag	UNP Q5SWA1
K	627	ALA	-	expression tag	UNP Q5SWA1
K	628	MET	-	expression tag	UNP Q5SWA1
K	629	ASP	-	expression tag	UNP Q5SWA1
K	630	PRO	-	expression tag	UNP Q5SWA1
K	702	LEU	-	expression tag	UNP Q5SWA1
K	703	GLU	-	expression tag	UNP Q5SWA1
K	704	HIS	-	expression tag	UNP Q5SWA1
K	705	HIS	-	expression tag	UNP Q5SWA1
K	706	HIS	-	expression tag	UNP Q5SWA1
K	707	HIS	-	expression tag	UNP Q5SWA1
K	708	HIS	-	expression tag	UNP Q5SWA1
K	709	HIS	-	expression tag	UNP Q5SWA1
O	626	GLY	-	expression tag	UNP Q5SWA1
O	627	ALA	-	expression tag	UNP Q5SWA1
O	628	MET	-	expression tag	UNP Q5SWA1
O	629	ASP	-	expression tag	UNP Q5SWA1
O	630	PRO	-	expression tag	UNP Q5SWA1
O	702	LEU	-	expression tag	UNP Q5SWA1
O	703	GLU	-	expression tag	UNP Q5SWA1
O	704	HIS	-	expression tag	UNP Q5SWA1
O	705	HIS	-	expression tag	UNP Q5SWA1
O	706	HIS	-	expression tag	UNP Q5SWA1
O	707	HIS	-	expression tag	UNP Q5SWA1
O	708	HIS	-	expression tag	UNP Q5SWA1
O	709	HIS	-	expression tag	UNP Q5SWA1

- Molecule 4 is LATRUNCULIN B (three-letter code: LAB) (formula: C₂₀H₂₉NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	L	1	Total	C	N	O	S	0	0
			27	20	1	5	1		
4	M	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

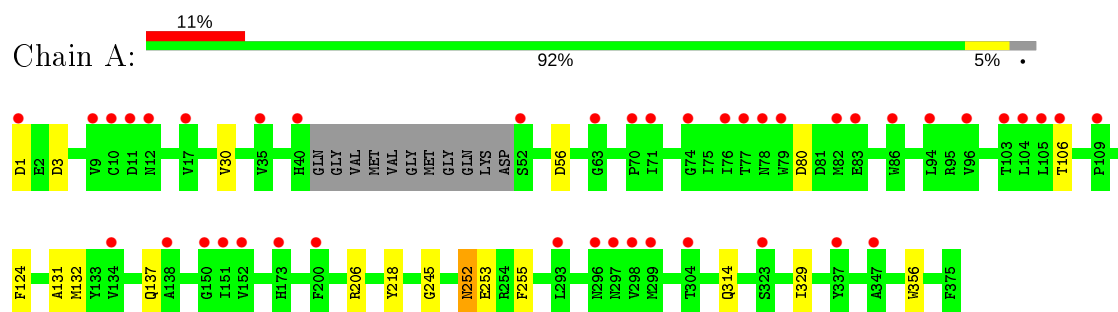
- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	2	Total	Mn	0	0
			2	2		
6	J	2	Total	Mn	0	0
			2	2		
6	D	2	Total	Mn	0	0
			2	2		
6	N	2	Total	Mn	0	0
			2	2		
6	F	2	Total	Mn	0	0
			2	2		

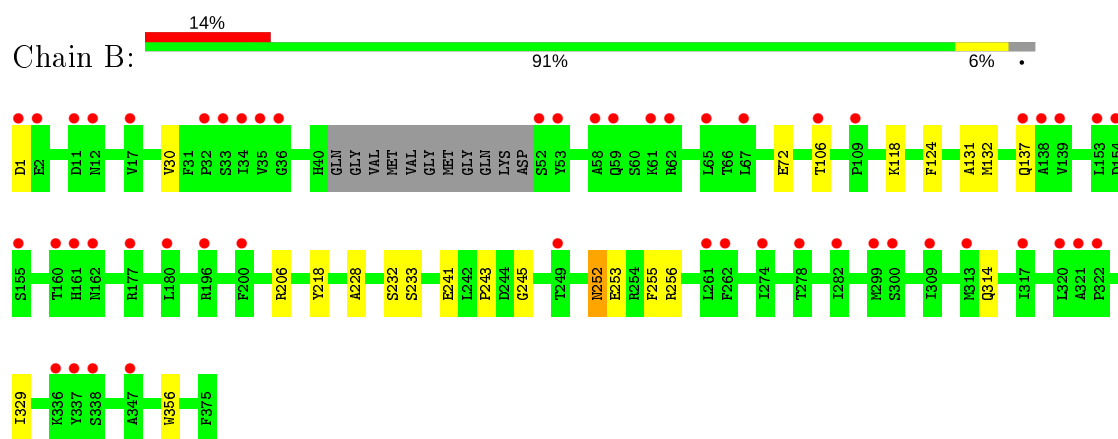
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

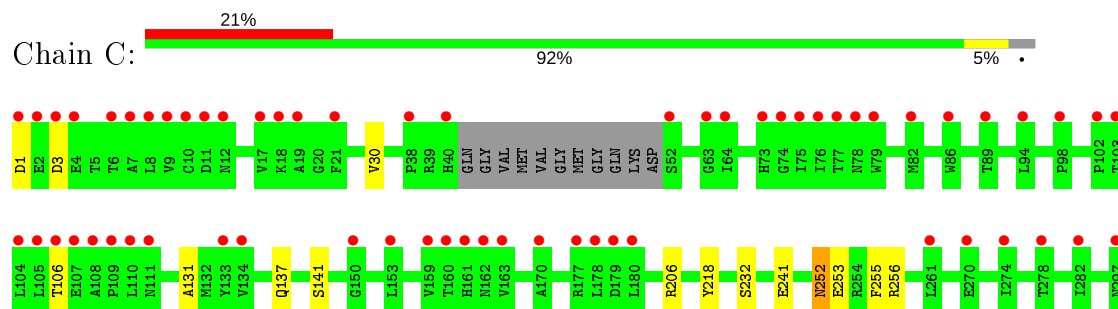
- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

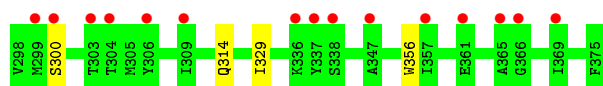


- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

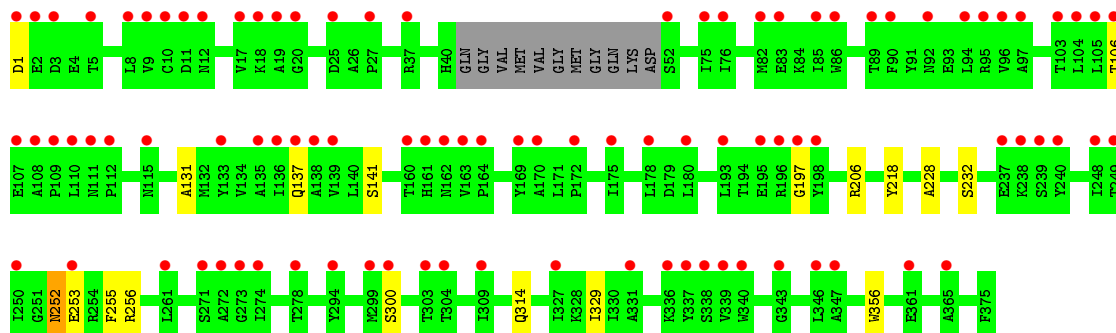
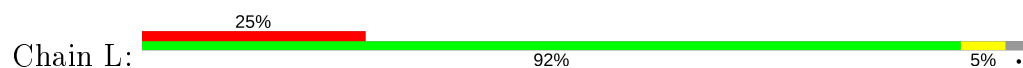


- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

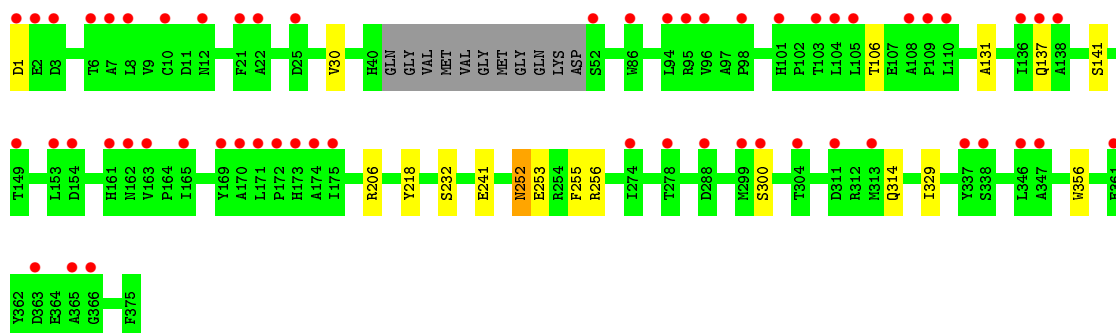




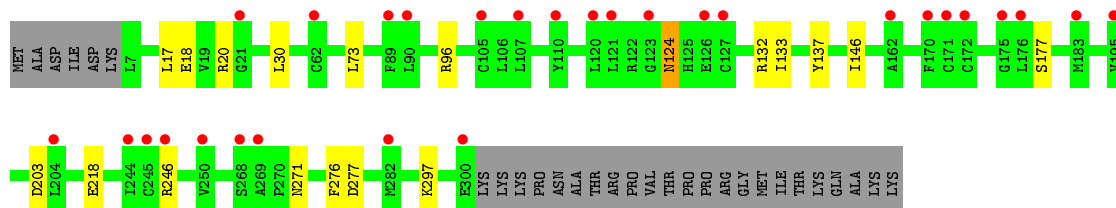
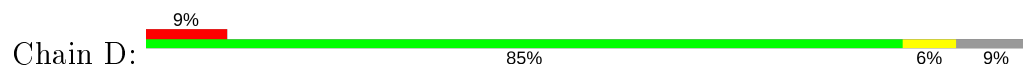
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



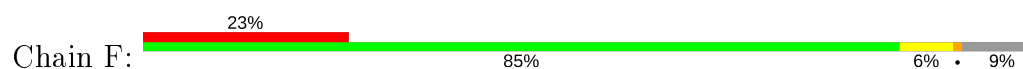
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

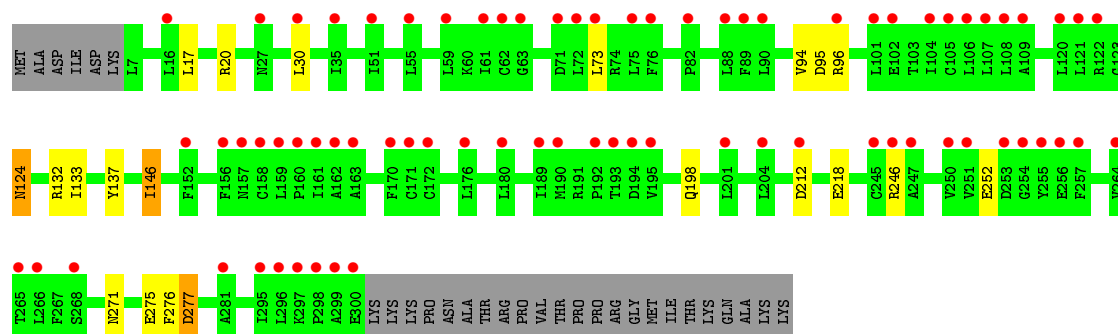


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

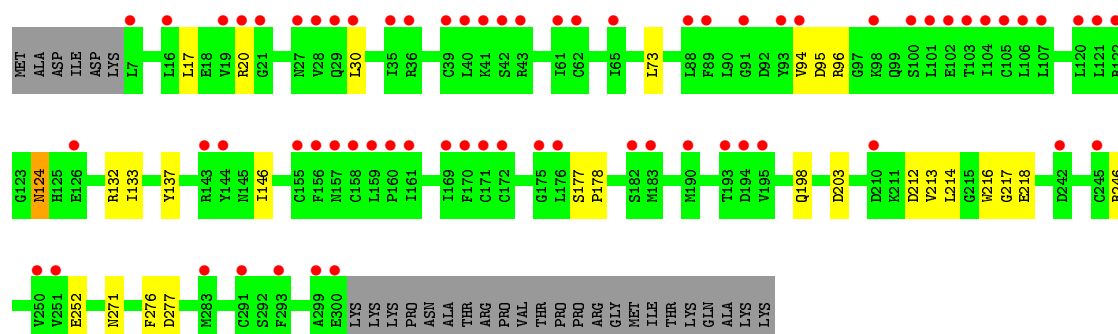
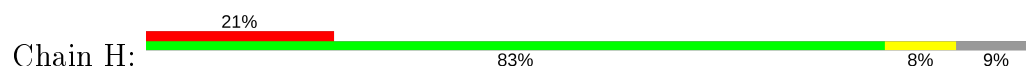


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

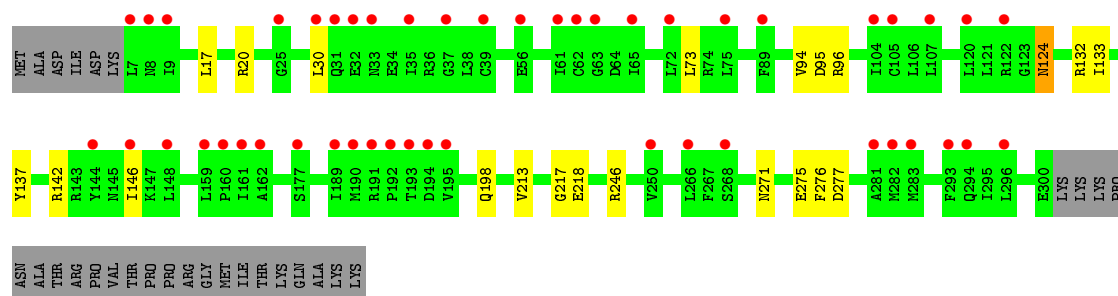
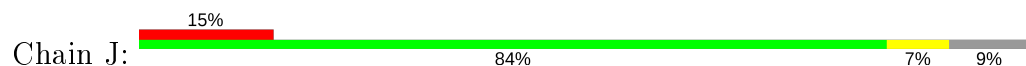




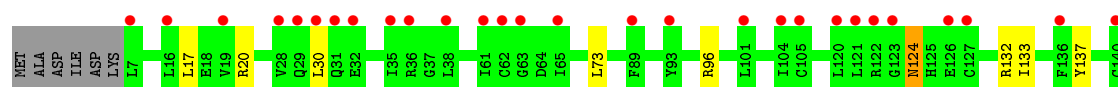
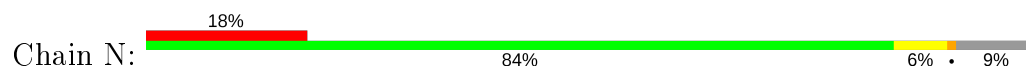
• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT

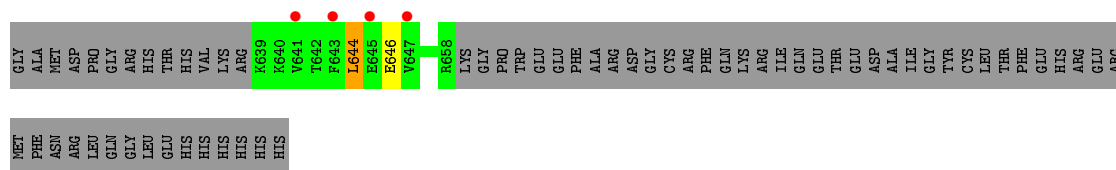


• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT



• Molecule 2: SERINE/THREONINE-PROTEIN PHOSPHATASE PP1-GAMMA CATALYTIC SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 149.93Å 318.72Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	82.79 – 7.88 82.79 – 7.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (82.79-7.88) 97.8 (82.79-7.88)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.370 , 0.400 0.354 , 0.375	Depositor DCC
R_{free} test set	290 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	356.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 456.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	27065	wwPDB-VP
Average B, all atoms (Å ²)	394.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, LAB, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2896	0.60	0/3927
1	B	0.47	0/2896	0.60	0/3927
1	C	0.46	0/2896	0.60	0/3927
1	L	0.47	0/2896	0.60	0/3927
1	M	0.47	0/2896	0.60	0/3927
2	D	0.29	0/2404	0.52	0/3250
2	F	0.30	0/2404	0.52	1/3250 (0.0%)
2	H	0.29	0/2404	0.52	0/3250
2	J	0.29	0/2404	0.52	0/3250
2	N	0.29	0/2404	0.52	1/3250 (0.0%)
3	E	0.37	0/169	0.59	0/226
3	G	0.31	0/169	0.56	0/226
3	I	0.32	0/169	0.56	0/226
3	K	0.31	0/169	0.55	0/226
3	O	0.31	0/169	0.56	0/226
All	All	0.39	0/27345	0.57	2/37015 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	146	ILE	CB-CA-C	-5.50	100.59	111.60
2	F	146	ILE	CB-CA-C	-5.34	100.93	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2835	0	2787	46	4
1	B	2835	0	2787	22	5
1	C	2835	0	2787	24	0
1	L	2835	0	2787	19	2
1	M	2835	0	2787	14	0
2	D	2351	0	2304	16	4
2	F	2351	0	2303	65	0
2	H	2351	0	2304	51	0
2	J	2351	0	2304	29	2
2	N	2351	0	2304	28	0
3	E	167	0	157	4	5
3	G	167	0	157	1	0
3	I	167	0	157	1	0
3	K	167	0	157	1	0
3	O	167	0	157	1	0
4	A	27	0	29	1	0
4	B	27	0	29	1	0
4	C	27	0	29	1	0
4	L	27	0	29	1	0
4	M	27	0	29	1	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
5	L	31	0	12	0	0
5	M	31	0	12	0	0
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	H	2	0	0	0	0
6	J	2	0	0	0	0
6	N	2	0	0	0	0
All	All	27065	0	26444	210	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:HB3	2:F:146:ILE:CG1	1.49	1.43
1:A:1:ASP:HB3	2:F:146:ILE:CD1	1.50	1.40
1:A:1:ASP:CB	2:F:146:ILE:CD1	2.02	1.35
1:A:1:ASP:CB	2:F:146:ILE:HD11	1.55	1.35
2:F:198:GLN:NE2	1:M:232:SER:O	1.61	1.33
2:J:142:ARG:NH1	1:L:197:GLY:HA2	1.47	1.28
1:C:232:SER:O	2:J:198:GLN:NE2	1.69	1.25
1:C:1:ASP:CG	2:H:137:TYR:OH	1.74	1.24
1:A:1:ASP:O	2:F:146:ILE:HG13	1.29	1.21
2:F:277:ASP:OD1	2:H:214:LEU:HB3	1.48	1.14
1:A:1:ASP:HB3	2:F:146:ILE:HG12	1.16	1.10
2:F:275:GLU:OE1	2:H:217:GLY:HA2	1.52	1.09
1:B:232:SER:O	2:H:198:GLN:NE2	1.87	1.08
1:C:1:ASP:HB3	2:H:146:ILE:HD11	1.37	1.06
1:A:1:ASP:HB2	2:F:146:ILE:HD11	1.32	1.05
1:A:1:ASP:O	2:F:146:ILE:CG1	2.05	1.04
1:M:1:ASP:OD2	2:N:137:TYR:OH	1.73	1.04
2:J:276:PHE:HA	2:N:212:ASP:O	1.60	1.00
2:J:142:ARG:CD	1:L:197:GLY:HA3	1.91	0.99
2:J:142:ARG:HD2	1:L:197:GLY:HA3	1.01	0.97
2:J:142:ARG:HH11	1:L:197:GLY:CA	1.80	0.95
2:J:142:ARG:HD2	1:L:197:GLY:CA	1.95	0.94
2:J:142:ARG:NH1	1:L:197:GLY:CA	2.32	0.93
1:A:1:ASP:C	2:F:146:ILE:HD11	1.89	0.92
1:A:1:ASP:CB	2:F:146:ILE:CG1	2.36	0.91
2:F:275:GLU:HB3	2:H:216:TRP:O	1.70	0.91
1:A:1:ASP:CA	2:F:146:ILE:HD11	2.02	0.90
1:A:1:ASP:CB	2:F:146:ILE:HG12	1.98	0.90
2:J:142:ARG:HH11	1:L:197:GLY:HA2	1.06	0.89
1:C:1:ASP:CG	2:H:137:TYR:HH	1.65	0.87
1:C:1:ASP:OD1	2:H:137:TYR:OH	1.95	0.84
2:J:271:ASN:ND2	2:J:276:PHE:O	2.12	0.82
1:A:3:ASP:CB	2:F:146:ILE:HD12	2.10	0.82
2:N:271:ASN:ND2	2:N:276:PHE:O	2.12	0.81
1:A:1:ASP:HB2	2:F:146:ILE:CD1	1.91	0.81
2:D:271:ASN:ND2	2:D:276:PHE:O	2.12	0.81
1:C:1:ASP:OD1	2:H:137:TYR:CE2	2.34	0.81
2:F:271:ASN:ND2	2:F:276:PHE:O	2.12	0.81
1:A:1:ASP:C	2:F:146:ILE:CD1	2.49	0.81
2:F:277:ASP:OD2	2:H:214:LEU:HD23	1.81	0.80
2:H:271:ASN:ND2	2:H:276:PHE:O	2.12	0.79
1:M:1:ASP:CG	2:N:137:TYR:OH	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:HB3	2:F:146:ILE:HD13	1.64	0.77
1:A:3:ASP:OD2	2:F:146:ILE:HD13	1.84	0.77
2:F:275:GLU:OE1	2:H:217:GLY:CA	2.31	0.76
2:J:275:GLU:OE1	2:N:217:GLY:HA2	1.86	0.76
1:C:1:ASP:OD1	2:H:137:TYR:CZ	2.41	0.73
2:J:275:GLU:CD	2:N:217:GLY:HA2	2.09	0.73
1:A:1:ASP:CB	2:F:146:ILE:HD13	2.15	0.72
1:A:3:ASP:HB3	2:F:146:ILE:HD12	1.72	0.72
1:A:1:ASP:O	2:F:146:ILE:CD1	2.38	0.70
2:F:252:GLU:HB3	2:H:212:ASP:OD1	1.94	0.67
2:D:297:LYS:HE2	3:E:651:TYR:OH	1.93	0.67
2:F:275:GLU:CB	2:H:216:TRP:O	2.41	0.67
2:F:277:ASP:OD1	2:H:214:LEU:CB	2.37	0.67
1:A:56:ASP:CG	1:B:243:PRO:O	2.33	0.67
1:A:3:ASP:OD2	2:F:146:ILE:HG21	1.96	0.66
1:A:1:ASP:C	2:F:146:ILE:CG1	2.65	0.65
1:A:3:ASP:N	2:F:146:ILE:HD12	2.13	0.64
1:A:3:ASP:CG	2:F:146:ILE:CD1	2.67	0.63
2:F:17:LEU:O	2:F:20:ARG:NH1	2.32	0.63
1:C:1:ASP:CB	2:H:146:ILE:HD11	2.22	0.63
2:N:17:LEU:O	2:N:20:ARG:NH1	2.32	0.63
2:D:297:LYS:HD3	3:E:651:TYR:CZ	2.32	0.63
2:D:17:LEU:O	2:D:20:ARG:NH1	2.31	0.63
2:J:275:GLU:OE1	2:N:217:GLY:CA	2.46	0.63
2:H:17:LEU:O	2:H:20:ARG:NH1	2.32	0.63
2:F:276:PHE:HA	2:H:213:VAL:HA	1.81	0.63
1:C:3:ASP:HB3	2:H:146:ILE:HD12	1.81	0.62
2:J:17:LEU:O	2:J:20:ARG:NH1	2.32	0.62
2:F:277:ASP:OD2	2:H:214:LEU:CD2	2.47	0.62
2:F:275:GLU:CD	2:H:217:GLY:HA2	2.19	0.62
1:M:1:ASP:OD1	2:N:137:TYR:OH	2.18	0.61
2:D:17:LEU:HB3	2:D:20:ARG:NH1	2.18	0.59
2:N:17:LEU:HB3	2:N:20:ARG:NH1	2.18	0.59
1:C:1:ASP:OD1	2:H:137:TYR:HE2	1.86	0.59
2:H:17:LEU:HB3	2:H:20:ARG:NH1	2.17	0.58
2:J:17:LEU:HB3	2:J:20:ARG:NH1	2.18	0.58
2:F:17:LEU:HB3	2:F:20:ARG:NH1	2.18	0.58
2:F:275:GLU:OE1	2:H:218:GLU:N	2.37	0.58
1:C:1:ASP:HB3	2:H:146:ILE:CD1	2.24	0.58
2:F:20:ARG:HG2	2:F:73:LEU:HD13	1.86	0.58
2:F:277:ASP:CG	2:H:214:LEU:HD23	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:ARG:HG2	2:N:73:LEU:HD13	1.86	0.58
2:J:20:ARG:HG2	2:J:73:LEU:HD13	1.86	0.57
2:D:20:ARG:HG2	2:D:73:LEU:HD13	1.86	0.57
1:C:30:VAL:O	1:M:241:GLU:OE2	2.23	0.57
2:J:218:GLU:N	2:N:275:GLU:OE1	2.36	0.57
1:A:1:ASP:CA	2:F:146:ILE:CG1	2.82	0.57
2:F:277:ASP:CG	2:H:214:LEU:HB3	2.23	0.56
1:B:1:ASP:OD2	2:D:146:ILE:HD11	2.05	0.56
2:H:20:ARG:HG2	2:H:73:LEU:HD13	1.86	0.56
1:C:241:GLU:OE2	1:M:30:VAL:O	2.24	0.55
1:A:3:ASP:CG	2:F:146:ILE:HD13	2.27	0.54
2:J:275:GLU:HB3	2:N:213:VAL:HG23	1.88	0.54
1:A:3:ASP:CG	2:F:146:ILE:HD12	2.28	0.54
1:A:30:VAL:O	1:B:241:GLU:OE2	2.26	0.53
2:N:218:GLU:OE1	2:N:218:GLU:HA	2.08	0.53
2:D:297:LYS:CE	3:E:651:TYR:OH	2.57	0.53
1:B:228:ALA:CB	2:H:178:PRO:HB2	2.39	0.53
2:J:217:GLY:HA2	2:N:275:GLU:OE1	2.09	0.53
2:N:17:LEU:HB3	2:N:20:ARG:HH12	1.74	0.53
2:D:17:LEU:HB3	2:D:20:ARG:HH12	1.74	0.53
2:H:124:ASN:HD22	2:H:124:ASN:H	1.57	0.53
2:F:124:ASN:H	2:F:124:ASN:HD22	1.57	0.52
1:C:3:ASP:OD2	2:H:146:ILE:CD1	2.57	0.52
2:D:124:ASN:HD22	2:D:124:ASN:H	1.57	0.52
2:F:17:LEU:HB3	2:F:20:ARG:HH12	1.74	0.52
2:J:218:GLU:HA	2:J:218:GLU:OE1	2.09	0.52
1:L:232:SER:HB3	2:N:225:PHE:HZ	1.75	0.52
2:J:217:GLY:HA2	2:N:275:GLU:CD	2.30	0.52
2:H:218:GLU:OE1	2:H:218:GLU:HA	2.10	0.52
2:N:124:ASN:HD22	2:N:124:ASN:H	1.57	0.51
2:H:17:LEU:HB3	2:H:20:ARG:HH12	1.74	0.51
2:F:275:GLU:HB3	2:H:217:GLY:HA2	1.91	0.51
2:J:124:ASN:HD22	2:J:124:ASN:H	1.57	0.51
2:F:277:ASP:CG	2:H:214:LEU:CD2	2.80	0.50
2:F:218:GLU:HA	2:F:218:GLU:OE1	2.10	0.50
2:J:17:LEU:HB3	2:J:20:ARG:HH12	1.74	0.50
1:L:232:SER:CB	2:N:225:PHE:HZ	2.24	0.50
1:B:228:ALA:HB3	2:H:178:PRO:HB2	1.92	0.50
2:D:218:GLU:HA	2:D:218:GLU:OE1	2.11	0.50
1:L:232:SER:HB3	2:N:225:PHE:CZ	2.48	0.48
1:A:56:ASP:HB3	1:B:243:PRO:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:277:ASP:CG	2:H:214:LEU:CB	2.82	0.47
1:C:1:ASP:CB	2:H:137:TYR:OH	2.59	0.47
2:F:275:GLU:O	2:H:214:LEU:O	2.33	0.47
2:J:275:GLU:O	2:N:213:VAL:HA	2.14	0.47
3:I:644:LEU:HD22	3:I:646:GLU:H	1.80	0.47
1:A:56:ASP:CB	1:B:243:PRO:O	2.62	0.47
1:B:252:ASN:HD22	1:B:253:GLU:N	2.13	0.47
2:F:275:GLU:CB	2:H:217:GLY:HA2	2.45	0.47
1:L:252:ASN:HD22	1:L:253:GLU:N	2.13	0.47
1:B:218:TYR:O	1:B:255:PHE:HA	2.15	0.47
1:M:218:TYR:O	1:M:255:PHE:HA	2.15	0.47
1:C:1:ASP:CG	2:H:137:TYR:CZ	2.77	0.46
1:A:252:ASN:HD22	1:A:253:GLU:N	2.13	0.46
1:C:252:ASN:HD22	1:C:253:GLU:N	2.13	0.46
1:L:218:TYR:O	1:L:255:PHE:HA	2.16	0.46
3:O:644:LEU:HD22	3:O:646:GLU:H	1.80	0.46
3:K:644:LEU:HD22	3:K:646:GLU:H	1.80	0.46
1:M:252:ASN:HD22	1:M:253:GLU:N	2.13	0.46
3:E:644:LEU:HD22	3:E:646:GLU:H	1.81	0.46
3:G:644:LEU:HD22	3:G:646:GLU:H	1.80	0.46
1:A:245:GLY:CA	1:B:30:VAL:O	2.64	0.46
2:J:213:VAL:HG23	2:N:275:GLU:O	2.16	0.46
1:C:218:TYR:O	1:C:255:PHE:HA	2.16	0.46
1:A:56:ASP:OD2	1:B:245:GLY:N	2.49	0.46
1:A:218:TYR:O	1:A:255:PHE:HA	2.15	0.45
2:F:275:GLU:CG	2:H:216:TRP:O	2.65	0.45
2:J:132:ARG:HA	2:J:137:TYR:HB2	1.99	0.45
2:N:146:ILE:HG21	2:N:146:ILE:HD13	1.74	0.45
1:A:245:GLY:HA2	1:B:30:VAL:O	2.17	0.45
1:L:206:ARG:HG2	4:L:1376:LAB:S1	2.57	0.44
1:A:314:GLN:OE1	1:A:329:ILE:HG12	2.18	0.44
2:J:132:ARG:NH2	2:J:133:ILE:HD11	2.33	0.44
1:L:314:GLN:OE1	1:L:329:ILE:HG12	2.18	0.44
2:N:132:ARG:HA	2:N:137:TYR:HB2	2.00	0.44
1:C:314:GLN:OE1	1:C:329:ILE:HG12	2.18	0.44
2:F:132:ARG:HA	2:F:137:TYR:HB2	1.99	0.44
2:H:132:ARG:NH2	2:H:133:ILE:HD11	2.33	0.44
1:A:3:ASP:OD2	2:F:146:ILE:CD1	2.62	0.44
1:B:233:SER:HB3	2:H:198:GLN:NE2	2.33	0.44
2:N:132:ARG:NH2	2:N:133:ILE:HD11	2.33	0.44
1:B:314:GLN:OE1	1:B:329:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:ARG:NH2	2:D:133:ILE:HD11	2.33	0.43
1:B:1:ASP:OD2	2:D:137:TYR:OH	2.36	0.43
1:B:131:ALA:HB1	1:B:356:TRP:HB3	2.01	0.43
2:F:146:ILE:HG21	2:F:146:ILE:HD13	1.74	0.43
2:H:132:ARG:HA	2:H:137:TYR:HB2	2.00	0.43
1:A:30:VAL:O	1:B:241:GLU:CD	2.57	0.43
2:F:212:ASP:OD1	2:H:252:GLU:HB3	2.19	0.43
1:M:314:GLN:OE1	1:M:329:ILE:HG12	2.18	0.43
1:B:206:ARG:HG2	4:B:1376:LAB:S1	2.59	0.43
2:F:132:ARG:NH2	2:F:133:ILE:HD11	2.33	0.43
2:J:275:GLU:O	2:N:214:LEU:N	2.41	0.43
1:C:206:ARG:HG2	4:C:1376:LAB:S1	2.59	0.43
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.42
2:H:146:ILE:HD13	2:H:146:ILE:HG21	1.76	0.42
1:L:131:ALA:HB1	1:L:356:TRP:HB3	2.01	0.42
1:C:131:ALA:HB1	1:C:356:TRP:HB3	2.00	0.42
2:F:252:GLU:CB	2:H:212:ASP:OD1	2.64	0.42
1:L:141:SER:HB3	1:L:300:SER:OG	2.20	0.42
2:D:132:ARG:HA	2:D:137:TYR:HB2	2.00	0.42
2:D:146:ILE:HD13	2:D:146:ILE:HG21	1.76	0.42
1:A:3:ASP:CA	2:F:146:ILE:HD12	2.49	0.42
1:M:206:ARG:HG2	4:M:1376:LAB:S1	2.59	0.42
1:C:106:THR:HB	1:C:137:GLN:HG3	2.02	0.42
1:A:206:ARG:HG2	4:A:1376:LAB:S1	2.60	0.42
1:M:141:SER:HB3	1:M:300:SER:OG	2.20	0.42
1:L:228:ALA:HB2	2:N:216:TRP:CD1	2.55	0.42
1:M:131:ALA:HB1	1:M:356:TRP:HB3	2.01	0.42
1:A:3:ASP:CB	2:F:146:ILE:CD1	2.90	0.41
1:B:106:THR:HB	1:B:137:GLN:HG3	2.02	0.41
2:H:94:VAL:O	2:H:95:ASP:HB2	2.21	0.41
1:L:252:ASN:ND2	1:L:256:ARG:HH11	2.19	0.41
1:C:252:ASN:ND2	1:C:256:ARG:HH11	2.19	0.41
1:A:3:ASP:HB3	2:F:146:ILE:CD1	2.47	0.41
1:B:252:ASN:ND2	1:B:256:ARG:HH11	2.19	0.41
2:J:94:VAL:O	2:J:95:ASP:HB2	2.21	0.41
2:D:177:SER:HB2	2:D:203:ASP:HB2	2.03	0.41
2:H:177:SER:HB2	2:H:203:ASP:HB2	2.03	0.41
1:A:106:THR:HB	1:A:137:GLN:HG3	2.02	0.41
2:F:94:VAL:O	2:F:95:ASP:HB2	2.21	0.41
1:L:106:THR:HB	1:L:137:GLN:HG3	2.02	0.41
1:M:106:THR:HB	1:M:137:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:ASN:ND2	1:M:256:ARG:HH11	2.19	0.41
1:C:141:SER:HB3	1:C:300:SER:OG	2.20	0.40
1:A:124:PHE:CZ	1:A:132:MET:HG3	2.57	0.40
1:B:124:PHE:CZ	1:B:132:MET:HG3	2.57	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:OD1	2:D:18:GLU:OE2[2_756]	1.24	0.96
2:J:137:TYR:OH	1:L:1:ASP:OD1[2_655]	1.30	0.90
1:B:72:GLU:OE2	3:E:646:GLU:OE1[4_756]	1.33	0.87
1:A:80:ASP:CG	2:D:18:GLU:OE2[2_756]	1.50	0.70
1:B:72:GLU:OE2	3:E:646:GLU:CD[4_756]	1.65	0.55
1:A:80:ASP:OD2	2:D:18:GLU:OE2[2_756]	1.68	0.52
2:J:146:ILE:CD1	1:L:1:ASP:CB[2_655]	1.69	0.51
1:A:80:ASP:OD1	2:D:18:GLU:CD[2_756]	2.00	0.20
1:B:118:LYS:NZ	3:E:651:TYR:CE1[4_756]	2.01	0.19
1:B:72:GLU:OE2	3:E:646:GLU:OE2[4_756]	2.02	0.18
1:B:118:LYS:NZ	3:E:651:TYR:CZ[4_756]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	B	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	C	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	L	360/375 (96%)	353 (98%)	7 (2%)	0	100	100
1	M	360/375 (96%)	353 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	F	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	H	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	J	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
2	N	292/323 (90%)	281 (96%)	11 (4%)	0	100	100
3	E	18/84 (21%)	18 (100%)	0	0	100	100
3	G	18/84 (21%)	18 (100%)	0	0	100	100
3	I	18/84 (21%)	18 (100%)	0	0	100	100
3	K	18/84 (21%)	18 (100%)	0	0	100	100
3	O	18/84 (21%)	18 (100%)	0	0	100	100
All	All	3350/3910 (86%)	3260 (97%)	90 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/318 (96%)	304 (100%)	1 (0%)	92	95
1	B	305/318 (96%)	304 (100%)	1 (0%)	92	95
1	C	305/318 (96%)	304 (100%)	1 (0%)	92	95
1	L	305/318 (96%)	304 (100%)	1 (0%)	92	95
1	M	305/318 (96%)	304 (100%)	1 (0%)	92	95
2	D	255/285 (90%)	250 (98%)	5 (2%)	55	74
2	F	255/285 (90%)	250 (98%)	5 (2%)	55	74
2	H	255/285 (90%)	250 (98%)	5 (2%)	55	74
2	J	255/285 (90%)	250 (98%)	5 (2%)	55	74
2	N	255/285 (90%)	250 (98%)	5 (2%)	55	74
3	E	18/74 (24%)	17 (94%)	1 (6%)	21	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	18/74 (24%)	17 (94%)	1 (6%)	21	46
3	I	18/74 (24%)	17 (94%)	1 (6%)	21	46
3	K	18/74 (24%)	17 (94%)	1 (6%)	21	46
3	O	18/74 (24%)	17 (94%)	1 (6%)	21	46
All	All	2890/3385 (85%)	2855 (99%)	35 (1%)	71	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	252	ASN
1	C	252	ASN
2	D	30	LEU
2	D	96	ARG
2	D	124	ASN
2	D	246	ARG
2	D	277	ASP
3	E	644	LEU
2	F	30	LEU
2	F	96	ARG
2	F	124	ASN
2	F	246	ARG
2	F	277	ASP
3	G	644	LEU
2	H	30	LEU
2	H	96	ARG
2	H	124	ASN
2	H	246	ARG
2	H	277	ASP
3	I	644	LEU
2	J	30	LEU
2	J	96	ARG
2	J	124	ASN
2	J	246	ARG
2	J	277	ASP
3	K	644	LEU
1	L	252	ASN
1	M	252	ASN
2	N	30	LEU
2	N	96	ARG
2	N	124	ASN

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Mol	Chain	Res	Type
2	N	246	ARG
2	N	277	ASP
3	O	644	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	88	HIS
1	A	252	ASN
1	A	280	ASN
1	B	59	GLN
1	B	88	HIS
1	B	252	ASN
1	B	280	ASN
1	C	59	GLN
1	C	88	HIS
1	C	252	ASN
1	C	280	ASN
2	J	198	GLN
1	L	59	GLN
1	L	88	HIS
1	L	252	ASN
1	L	280	ASN
1	M	59	GLN
1	M	88	HIS
1	M	252	ASN
1	M	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	M	1377	-	26,33,33	1.42	3 (11%)	31,52,52	1.25	1 (3%)
5	ATP	C	1377	-	26,33,33	1.43	3 (11%)	31,52,52	1.25	1 (3%)
5	ATP	B	1377	-	26,33,33	1.44	3 (11%)	31,52,52	1.24	1 (3%)
4	LAB	B	1376	-	28,29,29	4.52	8 (28%)	30,41,41	4.07	9 (30%)
5	ATP	A	1377	-	26,33,33	1.43	3 (11%)	31,52,52	1.24	1 (3%)
5	ATP	L	1377	-	26,33,33	1.43	3 (11%)	31,52,52	1.24	1 (3%)
4	LAB	L	1376	-	28,29,29	4.54	8 (28%)	30,41,41	4.07	9 (30%)
4	LAB	C	1376	-	28,29,29	4.54	8 (28%)	30,41,41	4.06	9 (30%)
4	LAB	A	1376	-	28,29,29	4.53	8 (28%)	30,41,41	4.07	9 (30%)
4	LAB	M	1376	-	28,29,29	4.54	8 (28%)	30,41,41	4.07	9 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	M	1377	-	-	1/18/38/38	0/3/3/3
5	ATP	C	1377	-	-	1/18/38/38	0/3/3/3
5	ATP	B	1377	-	-	1/18/38/38	0/3/3/3
4	LAB	B	1376	-	-	6/21/49/49	0/2/3/3
5	ATP	A	1377	-	-	1/18/38/38	0/3/3/3
5	ATP	L	1377	-	-	1/18/38/38	0/3/3/3
4	LAB	L	1376	-	-	6/21/49/49	0/2/3/3
4	LAB	C	1376	-	-	6/21/49/49	0/2/3/3
4	LAB	A	1376	-	-	6/21/49/49	0/2/3/3
4	LAB	M	1376	-	-	6/21/49/49	0/2/3/3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1376	LAB	C18-N1	13.21	1.51	1.34
4	M	1376	LAB	C18-N1	13.20	1.51	1.34
4	A	1376	LAB	C18-N1	13.18	1.51	1.34
4	C	1376	LAB	C18-N1	13.18	1.51	1.34
4	B	1376	LAB	C18-N1	13.01	1.51	1.34
4	M	1376	LAB	C2-C3	10.76	1.54	1.33
4	C	1376	LAB	C2-C3	10.75	1.54	1.33
4	B	1376	LAB	C2-C3	10.73	1.54	1.33
4	L	1376	LAB	C2-C3	10.73	1.54	1.33
4	A	1376	LAB	C2-C3	10.71	1.53	1.33
4	C	1376	LAB	O5-C18	8.78	1.35	1.22
4	B	1376	LAB	O5-C18	8.75	1.35	1.22
4	A	1376	LAB	O5-C18	8.73	1.35	1.22
4	L	1376	LAB	O5-C18	8.71	1.35	1.22
4	M	1376	LAB	O5-C18	8.70	1.35	1.22
4	B	1376	LAB	C17-S1	-8.15	1.64	1.81
4	C	1376	LAB	C17-S1	-8.12	1.64	1.81
4	M	1376	LAB	C17-S1	-8.09	1.64	1.81
4	A	1376	LAB	C17-S1	-8.09	1.64	1.81
4	L	1376	LAB	C17-S1	-8.06	1.64	1.81
4	L	1376	LAB	C16-N1	7.30	1.56	1.46
4	M	1376	LAB	C16-N1	7.30	1.56	1.46
4	C	1376	LAB	C16-N1	7.27	1.56	1.46
4	A	1376	LAB	C16-N1	7.26	1.56	1.46
4	B	1376	LAB	C16-N1	7.25	1.56	1.46
4	B	1376	LAB	C14-C13	-6.22	1.40	1.51
4	A	1376	LAB	C14-C13	-6.20	1.40	1.51
4	L	1376	LAB	C14-C13	-6.18	1.40	1.51
4	C	1376	LAB	C14-C13	-6.16	1.40	1.51
4	M	1376	LAB	C14-C13	-6.12	1.40	1.51
5	B	1377	ATP	C2'-C3'	-4.14	1.42	1.53
5	C	1377	ATP	C2'-C3'	-4.14	1.42	1.53
5	L	1377	ATP	C2'-C3'	-4.14	1.42	1.53
5	A	1377	ATP	C2'-C3'	-4.12	1.42	1.53
5	M	1377	ATP	C2'-C3'	-4.11	1.42	1.53
4	A	1376	LAB	C18-S1	-3.99	1.68	1.77
4	B	1376	LAB	C18-S1	-3.97	1.68	1.77
4	M	1376	LAB	C18-S1	-3.96	1.69	1.77
4	L	1376	LAB	C18-S1	-3.96	1.69	1.77
4	C	1376	LAB	C18-S1	-3.93	1.69	1.77
5	C	1377	ATP	C6-N6	3.47	1.46	1.34
5	A	1377	ATP	C6-N6	3.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1377	ATP	C6-N6	3.46	1.46	1.34
5	B	1377	ATP	C6-N6	3.45	1.46	1.34
4	M	1376	LAB	C17-C16	3.44	1.59	1.53
5	M	1377	ATP	C6-N6	3.43	1.46	1.34
4	C	1376	LAB	C17-C16	3.42	1.59	1.53
4	B	1376	LAB	C17-C16	3.41	1.59	1.53
4	A	1376	LAB	C17-C16	3.39	1.59	1.53
4	L	1376	LAB	C17-C16	3.37	1.59	1.53
5	M	1377	ATP	O4'-C4'	-2.11	1.40	1.45
5	B	1377	ATP	O4'-C4'	-2.09	1.40	1.45
5	C	1377	ATP	O4'-C4'	-2.09	1.40	1.45
5	L	1377	ATP	O4'-C4'	-2.09	1.40	1.45
5	A	1377	ATP	O4'-C4'	-2.07	1.40	1.45

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1376	LAB	O5-C18-N1	-19.17	105.88	126.81
4	B	1376	LAB	O5-C18-N1	-19.14	105.91	126.81
4	A	1376	LAB	O5-C18-N1	-19.13	105.92	126.81
4	M	1376	LAB	O5-C18-N1	-19.12	105.93	126.81
4	C	1376	LAB	O5-C18-N1	-19.11	105.94	126.81
4	M	1376	LAB	C17-S1-C18	7.28	95.91	92.00
4	A	1376	LAB	C17-S1-C18	7.21	95.87	92.00
4	B	1376	LAB	C17-S1-C18	7.19	95.86	92.00
4	L	1376	LAB	C17-S1-C18	7.18	95.85	92.00
4	C	1376	LAB	C17-S1-C18	7.14	95.83	92.00
5	B	1377	ATP	N3-C2-N1	-4.08	122.31	128.68
4	M	1376	LAB	C19-C3-C2	-4.05	110.59	122.77
4	C	1376	LAB	C19-C3-C2	-4.05	110.59	122.77
5	M	1377	ATP	N3-C2-N1	-4.05	122.35	128.68
5	C	1377	ATP	N3-C2-N1	-4.04	122.36	128.68
4	L	1376	LAB	C19-C3-C2	-4.04	110.63	122.77
5	A	1377	ATP	N3-C2-N1	-4.04	122.37	128.68
5	L	1377	ATP	N3-C2-N1	-4.03	122.37	128.68
4	A	1376	LAB	C19-C3-C2	-4.03	110.65	122.77
4	B	1376	LAB	C19-C3-C2	-4.03	110.65	122.77
4	M	1376	LAB	O2-C1-C2	3.41	119.28	111.27
4	L	1376	LAB	O2-C1-C2	3.40	119.25	111.27
4	B	1376	LAB	O2-C1-C2	3.40	119.24	111.27
4	C	1376	LAB	O2-C1-C2	3.39	119.22	111.27
4	A	1376	LAB	O2-C1-C2	3.38	119.21	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1376	LAB	C10-C9-C8	2.96	118.87	113.95
4	L	1376	LAB	C10-C9-C8	2.95	118.85	113.95
4	B	1376	LAB	C10-C9-C8	2.94	118.85	113.95
4	M	1376	LAB	C10-C9-C8	2.94	118.84	113.95
4	C	1376	LAB	C10-C9-C8	2.91	118.80	113.95
4	C	1376	LAB	C5-C4-C3	2.68	121.79	112.98
4	M	1376	LAB	C5-C4-C3	2.67	121.77	112.98
4	A	1376	LAB	C5-C4-C3	2.66	121.74	112.98
4	B	1376	LAB	C5-C4-C3	2.66	121.73	112.98
4	L	1376	LAB	C5-C4-C3	2.66	121.73	112.98
4	L	1376	LAB	O1-C1-C2	-2.34	120.32	126.23
4	M	1376	LAB	O1-C1-C2	-2.34	120.34	126.23
4	C	1376	LAB	O1-C1-C2	-2.33	120.37	126.23
4	A	1376	LAB	O1-C1-C2	-2.32	120.37	126.23
4	B	1376	LAB	O1-C1-C2	-2.32	120.37	126.23
4	B	1376	LAB	C19-C3-C4	-2.19	111.58	115.27
4	C	1376	LAB	C19-C3-C4	-2.19	111.59	115.27
4	L	1376	LAB	C19-C3-C4	-2.18	111.60	115.27
4	A	1376	LAB	C19-C3-C4	-2.18	111.61	115.27
4	M	1376	LAB	C19-C3-C4	-2.17	111.62	115.27
4	M	1376	LAB	C13-O2-C1	2.05	122.81	117.27
4	L	1376	LAB	C13-O2-C1	2.05	122.81	117.27
4	B	1376	LAB	C13-O2-C1	2.04	122.78	117.27
4	A	1376	LAB	C13-O2-C1	2.04	122.77	117.27
4	C	1376	LAB	C13-O2-C1	2.03	122.75	117.27

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1376	LAB	O3-C15-C16-C17
4	B	1376	LAB	C5-C6-C7-C8
4	B	1376	LAB	C1-C2-C3-C4
4	L	1376	LAB	O3-C15-C16-C17
4	L	1376	LAB	C5-C6-C7-C8
4	L	1376	LAB	C1-C2-C3-C4
4	C	1376	LAB	O3-C15-C16-C17
4	C	1376	LAB	C5-C6-C7-C8
4	C	1376	LAB	C1-C2-C3-C4
4	A	1376	LAB	O3-C15-C16-C17
4	A	1376	LAB	C5-C6-C7-C8
4	A	1376	LAB	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	M	1376	LAB	O3-C15-C16-C17
4	M	1376	LAB	C5-C6-C7-C8
4	M	1376	LAB	C1-C2-C3-C4
4	B	1376	LAB	C1-C2-C3-C19
4	L	1376	LAB	C1-C2-C3-C19
4	C	1376	LAB	C1-C2-C3-C19
4	A	1376	LAB	C1-C2-C3-C19
4	M	1376	LAB	C1-C2-C3-C19
4	B	1376	LAB	O2-C1-C2-C3
4	L	1376	LAB	O2-C1-C2-C3
4	C	1376	LAB	O2-C1-C2-C3
4	A	1376	LAB	O2-C1-C2-C3
4	M	1376	LAB	O2-C1-C2-C3
4	B	1376	LAB	O1-C1-C2-C3
4	L	1376	LAB	O1-C1-C2-C3
4	C	1376	LAB	O1-C1-C2-C3
4	A	1376	LAB	O1-C1-C2-C3
4	M	1376	LAB	O1-C1-C2-C3
5	M	1377	ATP	PG-O3B-PB-O1B
5	C	1377	ATP	PG-O3B-PB-O1B
5	B	1377	ATP	PG-O3B-PB-O1B
5	A	1377	ATP	PG-O3B-PB-O1B
5	L	1377	ATP	PG-O3B-PB-O1B

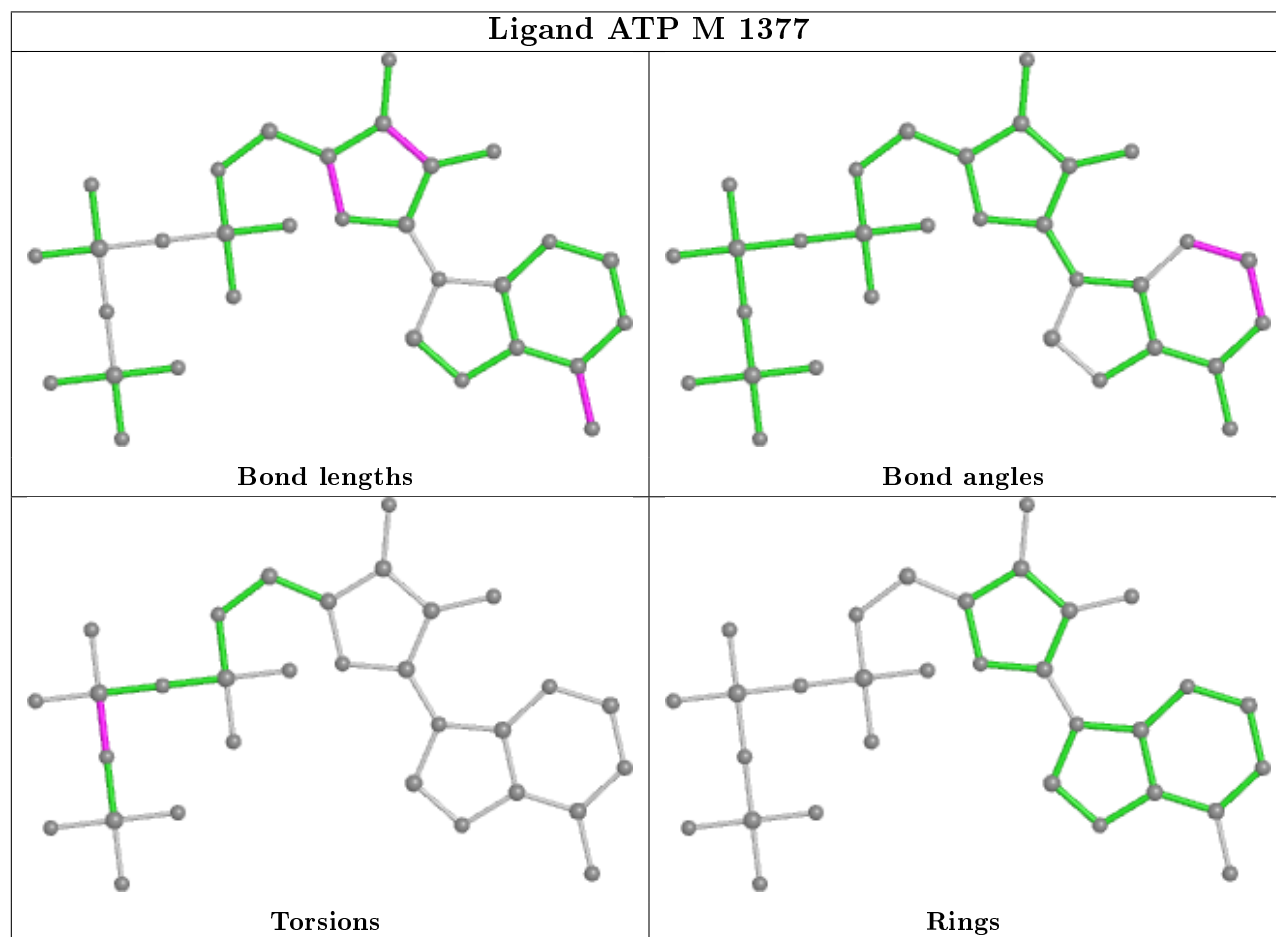
There are no ring outliers.

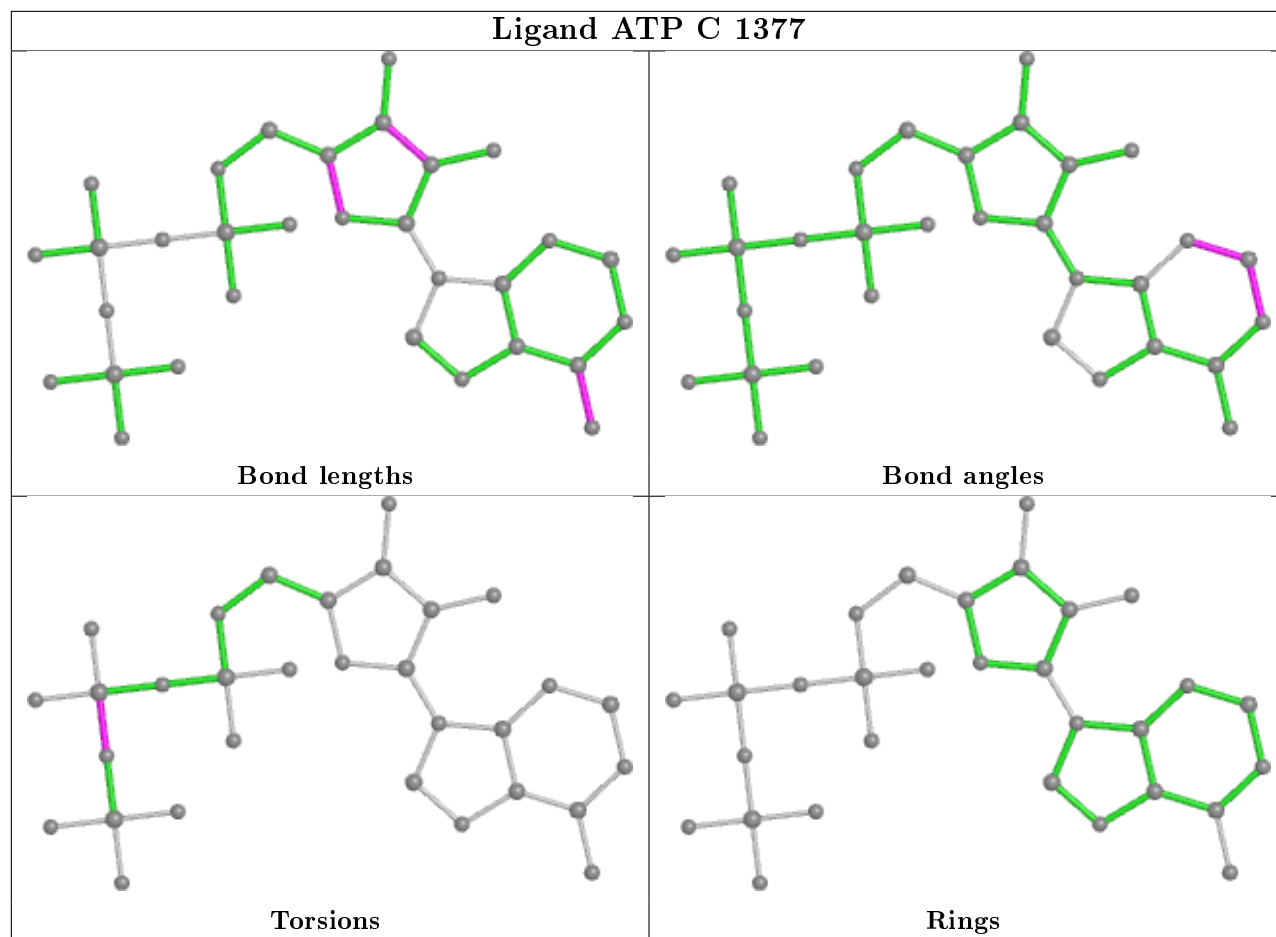
5 monomers are involved in 5 short contacts:

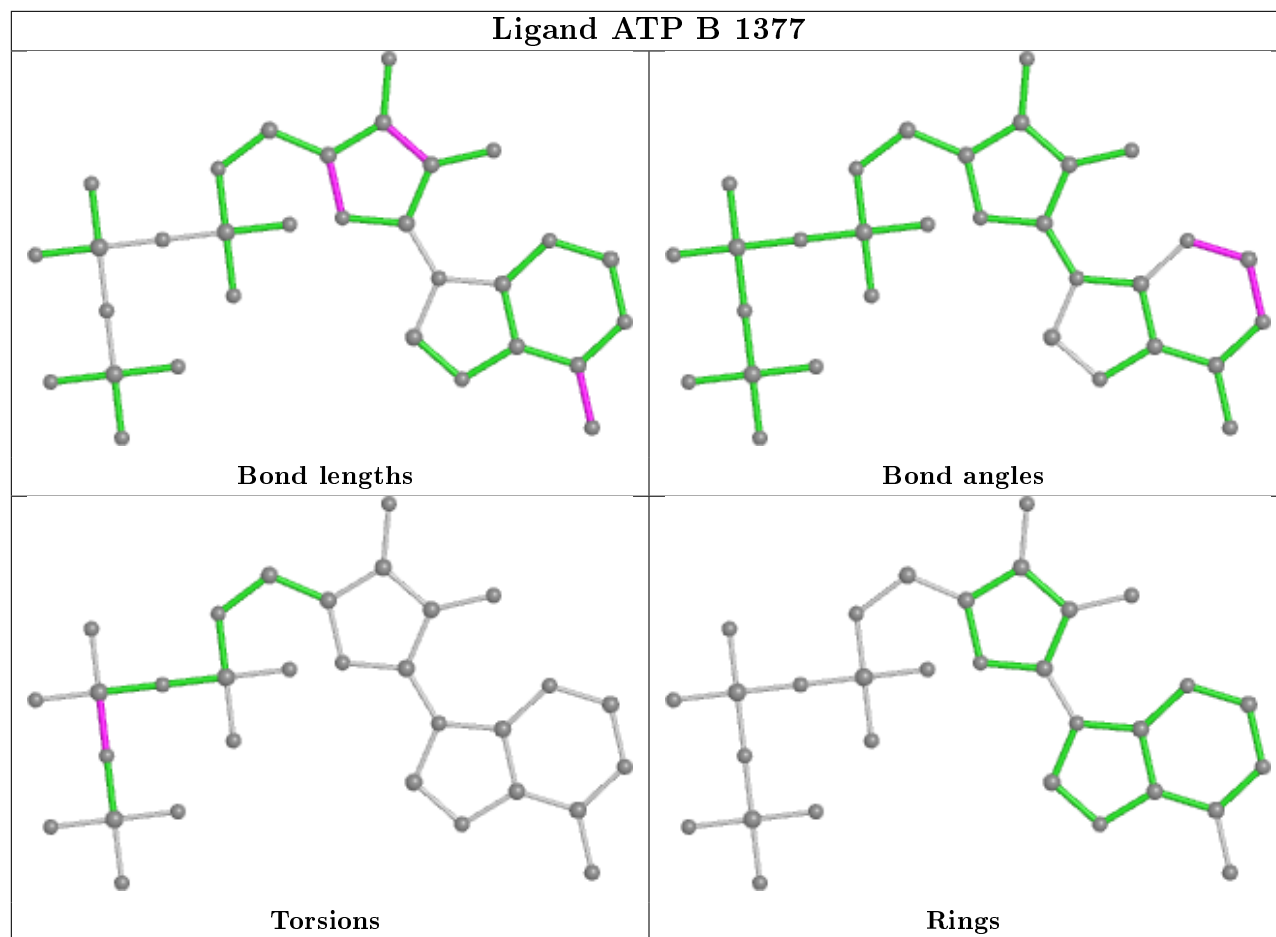
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1376	LAB	1	0
4	L	1376	LAB	1	0
4	C	1376	LAB	1	0
4	A	1376	LAB	1	0
4	M	1376	LAB	1	0

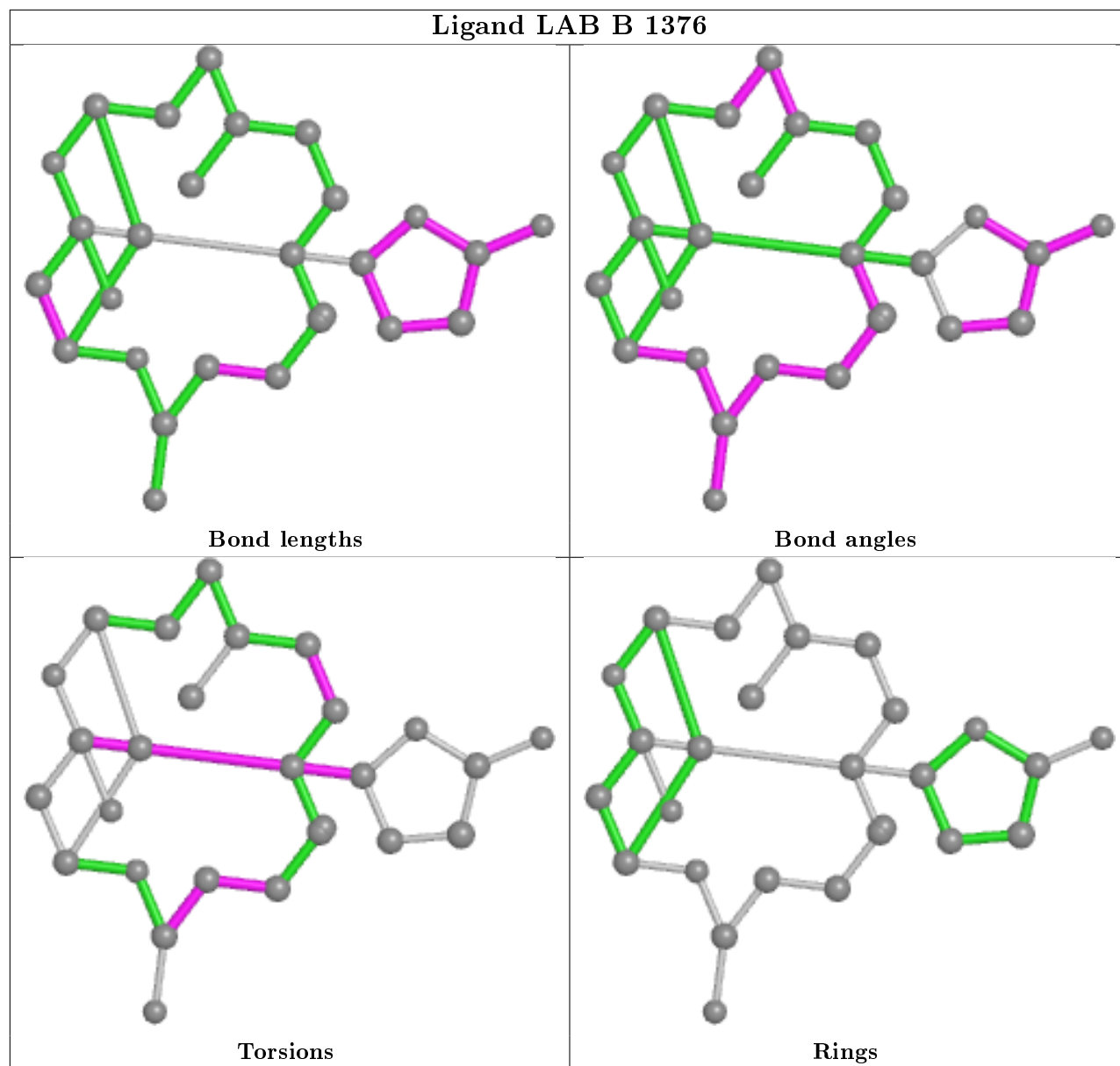
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

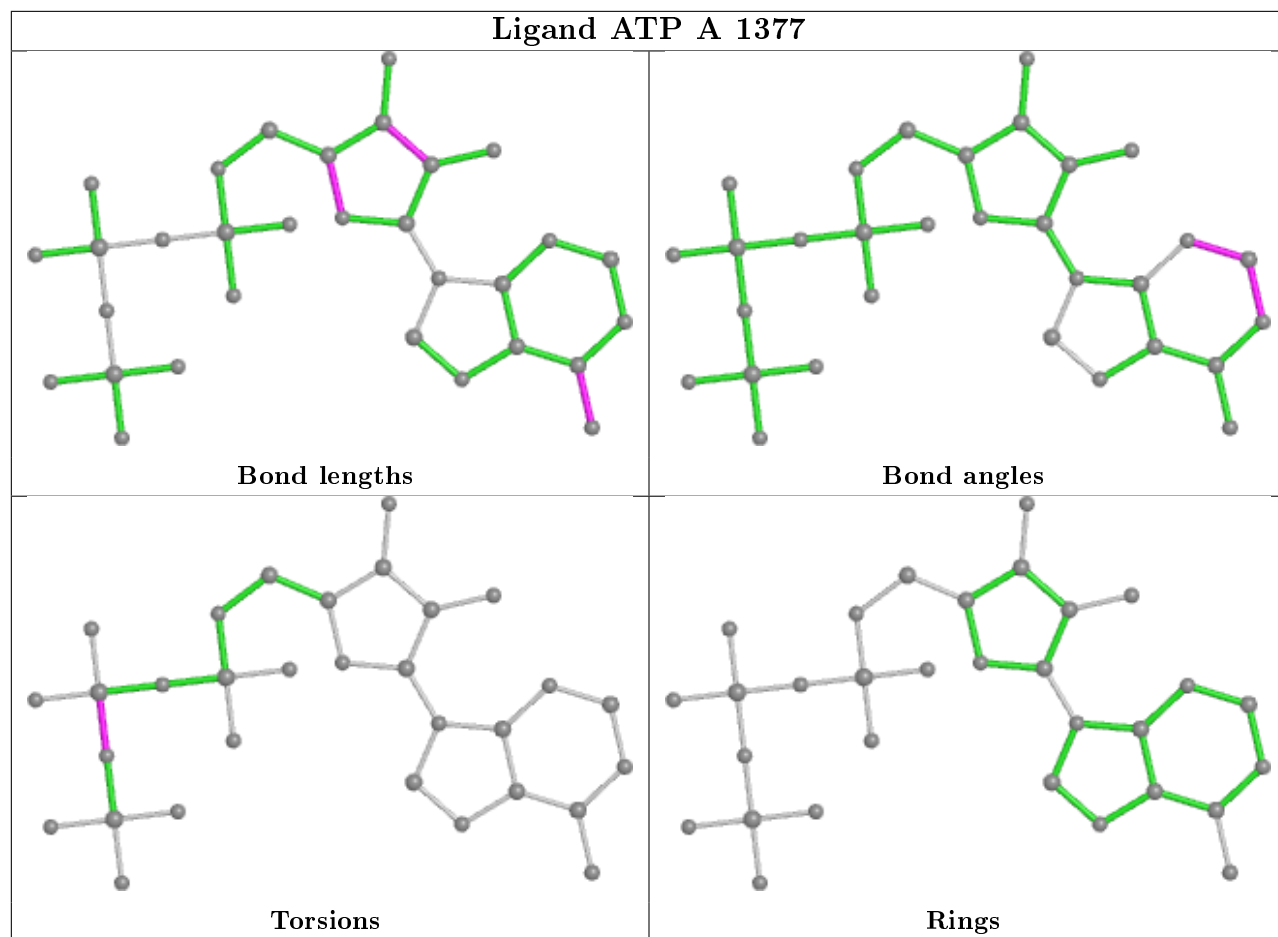
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

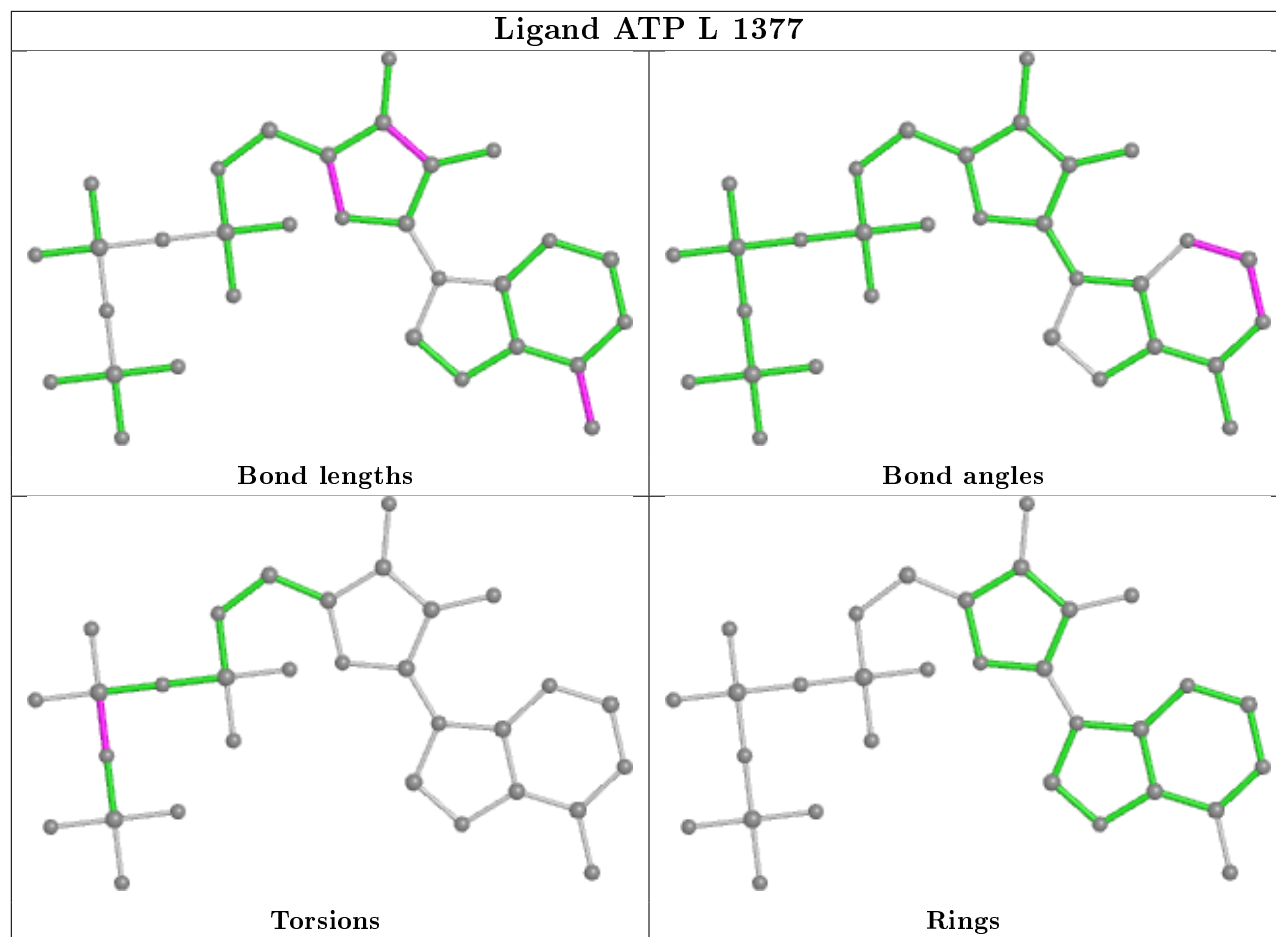


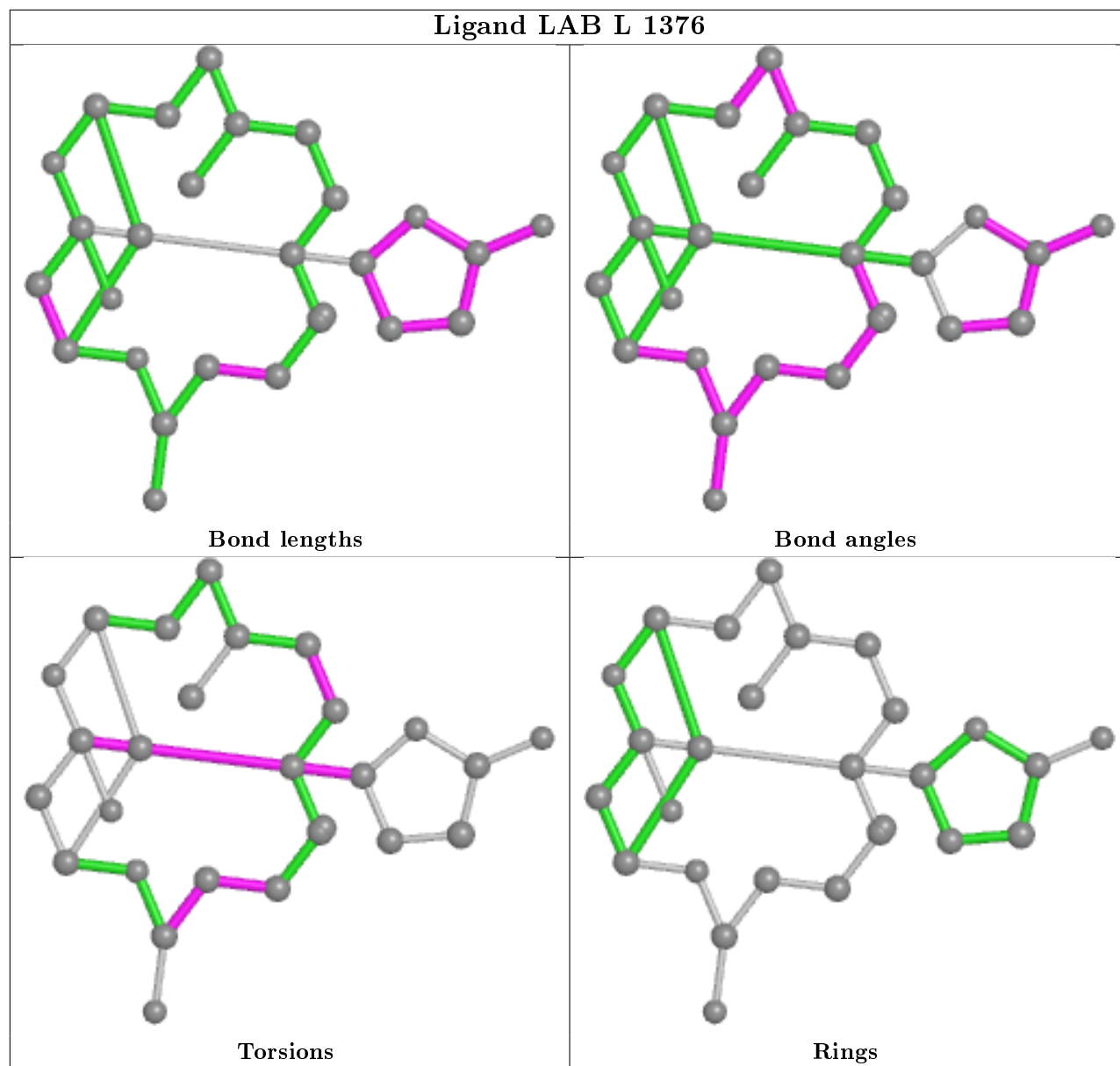


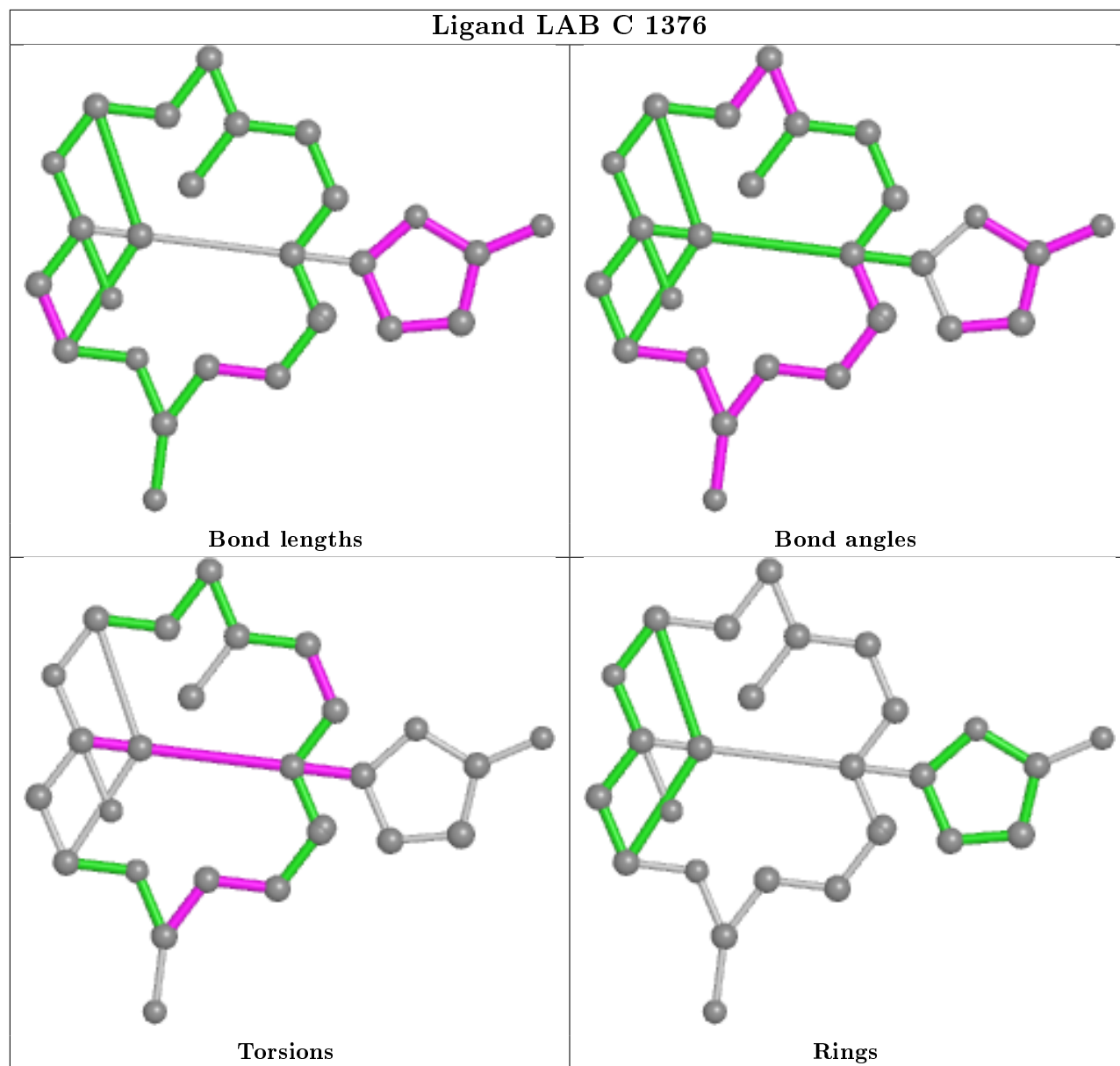




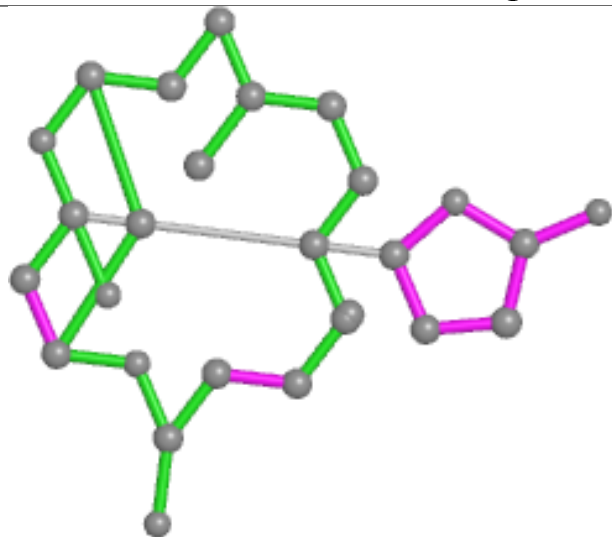




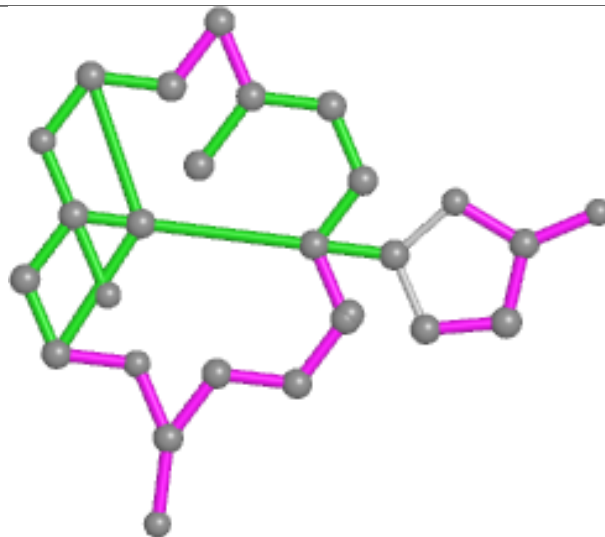




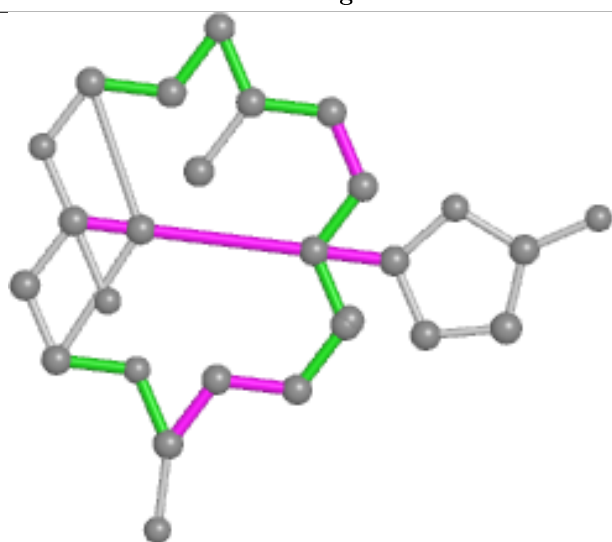
Ligand LAB A 1376



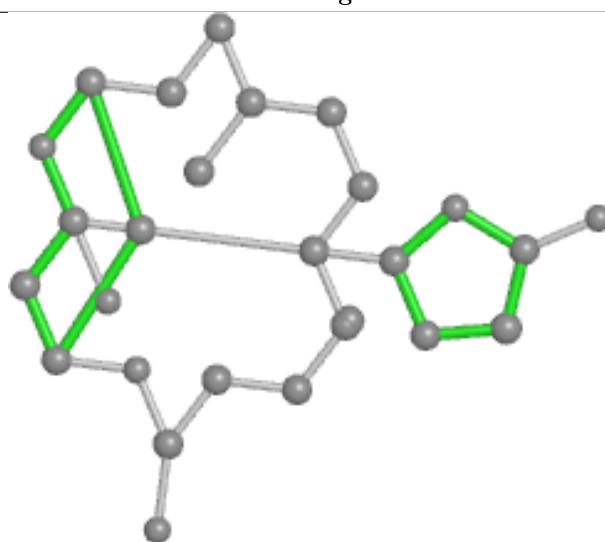
Bond lengths



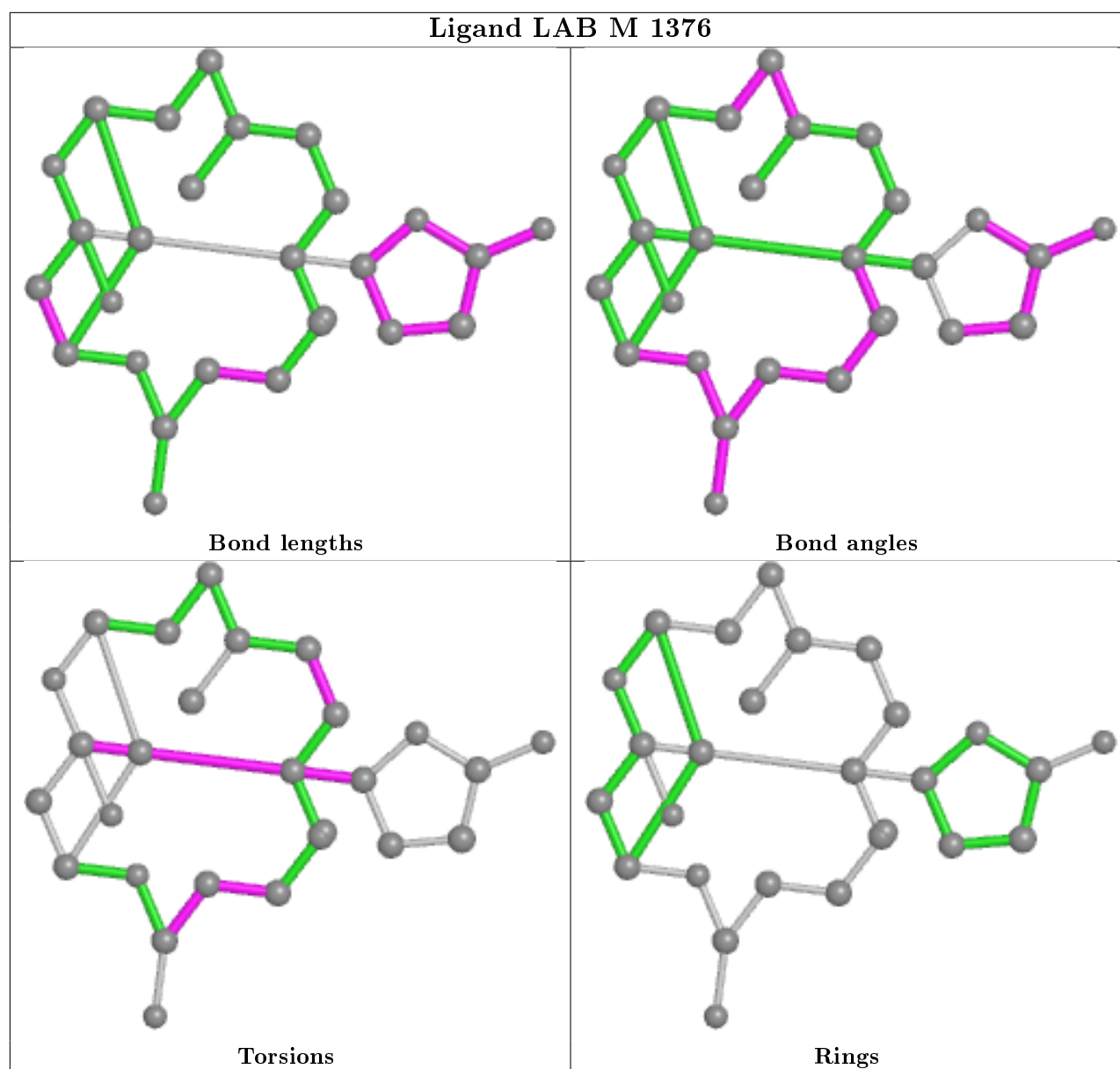
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/375 (97%)	0.86	43 (11%) 4 8	237, 303, 352, 385	0
1	B	364/375 (97%)	1.00	51 (14%) 2 6	252, 327, 380, 404	0
1	C	364/375 (97%)	1.26	77 (21%) 0 3	356, 410, 453, 502	0
1	L	364/375 (97%)	1.44	95 (26%) 0 2	403, 490, 565, 619	0
1	M	364/375 (97%)	0.99	57 (15%) 2 5	454, 521, 589, 621	0
2	D	294/323 (91%)	0.75	29 (9%) 7 10	232, 291, 334, 368	0
2	F	294/323 (91%)	1.28	75 (25%) 0 2	303, 364, 419, 450	0
2	H	294/323 (91%)	1.23	68 (23%) 0 2	311, 382, 436, 457	0
2	J	294/323 (91%)	0.93	48 (16%) 1 4	303, 367, 432, 478	0
2	N	294/323 (91%)	1.07	57 (19%) 1 3	285, 372, 419, 450	0
3	E	20/84 (23%)	0.76	1 (5%) 28 28	446, 573, 869, 969	0
3	G	20/84 (23%)	2.15	9 (45%) 0 1	497, 563, 717, 732	0
3	I	20/84 (23%)	1.86	8 (40%) 0 1	583, 761, 1000, 1000	0
3	K	20/84 (23%)	0.80	1 (5%) 28 28	471, 544, 652, 721	0
3	O	20/84 (23%)	0.77	4 (20%) 1 3	644, 682, 763, 789	0
All	All	3390/3910 (86%)	1.09	623 (18%) 1 4	232, 377, 559, 1000	0

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	109	PRO	14.5
1	L	108	ALA	12.1
2	N	194	ASP	11.0
1	C	10	CYS	9.8
2	D	172	CYS	9.4
1	M	109	PRO	8.7
2	F	265	THR	8.7

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Mol	Chain	Res	Type	RSRZ
1	C	12	ASN	7.7
2	N	193	THR	7.7
2	F	172	CYS	7.6
2	J	194	ASP	7.2
1	M	2	GLU	7.1
2	H	28	VAL	6.7
1	C	11	ASP	6.6
1	L	137	GLN	6.5
2	F	266	LEU	6.4
1	L	110	LEU	6.3
1	L	136	ILE	6.2
1	C	74	GLY	6.1
1	M	6	THR	6.1
1	C	109	PRO	6.1
2	F	62	CYS	6.0
1	L	96	VAL	6.0
1	C	105	LEU	6.0
2	F	105	CYS	6.0
1	L	239	SER	6.0
1	C	1	ASP	5.9
1	L	10	CYS	5.7
2	F	162	ALA	5.7
2	F	171	CYS	5.7
1	M	7	ALA	5.6
2	F	63	GLY	5.6
2	N	157	ASN	5.6
1	C	2	GLU	5.5
2	H	194	ASP	5.5
1	L	111	ASN	5.5
2	F	161	ILE	5.5
2	F	163	ALA	5.4
1	L	107	GLU	5.3
1	L	86	TRP	5.3
1	L	12	ASN	5.2
2	F	90	LEU	5.2
1	M	108	ALA	5.2
2	H	93	TYR	5.1
2	F	268	SER	5.1
2	H	104	ILE	5.1
2	F	250	VAL	5.1
2	N	161	ILE	5.0
2	F	245	CYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	M	138	ALA	5.0
1	L	82	MET	5.0
1	C	76	ILE	5.0
3	G	649	GLU	5.0
2	H	105	CYS	5.0
2	H	250	VAL	4.9
3	I	643	PHE	4.9
1	L	94	LEU	4.9
2	J	193	THR	4.8
1	M	96	VAL	4.8
1	B	138	ALA	4.8
1	C	179	ASP	4.8
2	J	250	VAL	4.8
1	A	150	GLY	4.8
1	L	271	SER	4.7
2	F	299	ALA	4.7
2	N	122	ARG	4.7
3	G	650	TYR	4.7
2	H	120	LEU	4.7
2	H	94	VAL	4.7
2	F	300	GLU	4.7
2	H	172	CYS	4.7
2	F	297	LYS	4.6
2	F	61	ILE	4.6
1	L	197	GLY	4.6
2	N	105	CYS	4.6
1	B	12	ASN	4.6
2	F	160	PRO	4.6
2	H	101	LEU	4.6
1	C	75	ILE	4.6
1	C	7	ALA	4.6
2	H	195	VAL	4.5
1	L	90	PHE	4.5
1	B	36	GLY	4.5
2	H	100	SER	4.5
1	B	109	PRO	4.5
2	D	171	CYS	4.5
1	M	103	THR	4.4
2	F	255	TYR	4.4
2	H	29	GLN	4.4
1	L	106	THR	4.4
1	A	12	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	175	GLY	4.4
1	C	161	HIS	4.4
2	N	62	CYS	4.4
2	F	104	ILE	4.4
2	N	171	CYS	4.4
1	L	337	TYR	4.4
2	J	35	ILE	4.4
1	C	177	ARG	4.3
1	L	89	THR	4.3
1	L	248	ILE	4.3
2	N	195	VAL	4.3
3	G	651	TYR	4.3
1	M	172	PRO	4.3
2	N	126	GLU	4.3
1	L	170	ALA	4.3
1	L	76	ILE	4.3
1	C	160	THR	4.3
2	N	28	VAL	4.3
2	D	245	CYS	4.3
1	L	196	ARG	4.3
2	F	256	GLU	4.2
2	F	193	THR	4.2
1	C	178	LEU	4.2
2	H	122	ARG	4.2
2	N	156	PHE	4.2
1	M	8	LEU	4.2
2	N	162	ALA	4.2
1	L	8	LEU	4.1
1	C	8	LEU	4.1
2	F	195	VAL	4.1
1	C	77	THR	4.1
2	H	193	THR	4.1
1	L	195	GLU	4.1
1	B	161	HIS	4.1
1	L	52	SER	4.1
1	M	299	MET	4.0
3	G	652	ILE	4.0
2	F	106	LEU	4.0
1	C	106	THR	4.0
1	A	52	SER	4.0
1	B	1	ASP	4.0
1	L	11	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	M	173	HIS	3.9
2	H	121	LEU	3.9
1	L	178	LEU	3.9
2	H	27	ASN	3.9
3	G	654	GLY	3.8
2	N	192	PRO	3.8
1	L	365	ALA	3.8
2	N	29	GLN	3.8
1	B	52	SER	3.8
2	N	30	LEU	3.8
2	H	39	CYS	3.8
1	M	10	CYS	3.8
3	G	653	SER	3.8
1	C	365	ALA	3.8
2	N	163	ALA	3.8
1	M	153	LEU	3.8
1	A	76	ILE	3.8
1	M	347	ALA	3.8
1	C	104	LEU	3.8
1	L	303	THR	3.7
2	F	257	PHE	3.7
1	M	365	ALA	3.7
2	J	282	MET	3.7
1	L	304	THR	3.7
1	C	304	THR	3.7
1	M	21	PHE	3.7
1	M	170	ALA	3.7
1	C	52	SER	3.7
1	C	366	GLY	3.7
1	L	104	LEU	3.7
1	L	180	LEU	3.6
1	M	300	SER	3.6
1	C	73	HIS	3.6
1	C	303	THR	3.6
2	N	152	PHE	3.6
1	L	300	SER	3.6
2	J	268	SER	3.6
2	N	268	SER	3.6
1	M	104	LEU	3.6
1	B	35	VAL	3.6
1	C	103	THR	3.6
1	M	337	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	264	VAL	3.6
1	M	304	THR	3.6
2	J	161	ILE	3.6
1	L	17	VAL	3.6
1	M	288	ASP	3.6
2	F	89	PHE	3.6
1	A	70	PRO	3.6
2	N	155	CYS	3.6
3	K	639	LYS	3.5
2	F	296	LEU	3.5
1	C	309	ILE	3.5
3	I	641	VAL	3.5
2	N	283	MET	3.5
2	H	245	CYS	3.5
1	L	19	ALA	3.5
1	A	106	THR	3.5
2	F	281	ALA	3.5
1	L	250	ILE	3.5
1	L	274	ILE	3.4
2	N	35	ILE	3.4
2	H	156	PHE	3.4
1	B	2	GLU	3.4
1	M	1	ASP	3.4
1	B	300	SER	3.4
1	B	337	TYR	3.4
1	L	25	ASP	3.4
1	A	40	HIS	3.4
1	B	154	ASP	3.4
2	H	7	LEU	3.4
2	F	251	VAL	3.4
1	A	35	VAL	3.4
2	H	103	THR	3.4
2	F	194	ASP	3.4
1	L	339	VAL	3.3
1	L	9	VAL	3.3
1	C	337	TYR	3.3
1	L	249	THR	3.3
1	L	95	ARG	3.3
2	H	102	GLU	3.3
1	M	3	ASP	3.3
2	F	158	CYS	3.3
2	J	65	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	189	ILE	3.3
2	N	7	LEU	3.3
2	N	16	LEU	3.3
2	H	299	ALA	3.3
1	L	193	LEU	3.3
2	N	153	THR	3.2
2	H	89	PHE	3.2
2	F	120	LEU	3.2
2	J	105	CYS	3.2
1	L	163	VAL	3.2
2	H	291	CYS	3.2
1	M	274	ILE	3.2
2	F	246	ARG	3.2
1	B	153	LEU	3.2
1	M	171	LEU	3.2
2	J	62	CYS	3.2
2	N	159	LEU	3.2
1	L	138	ALA	3.2
2	N	61	ILE	3.2
2	N	282	MET	3.2
2	N	144	TYR	3.2
1	B	53	TYR	3.2
1	C	6	THR	3.1
1	M	110	LEU	3.1
3	G	655	ASP	3.1
1	L	1	ASP	3.1
1	A	105	LEU	3.1
1	A	10	CYS	3.1
1	C	299	MET	3.1
2	D	175	GLY	3.1
2	H	35	ILE	3.1
2	J	195	VAL	3.1
2	F	27	ASN	3.1
1	L	299	MET	3.1
1	M	95	ARG	3.1
2	J	160	PRO	3.1
1	M	169	TYR	3.1
2	J	32	GLU	3.1
1	L	164	PRO	3.1
2	F	107	LEU	3.1
2	N	190	MET	3.1
3	G	656	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	346	LEU	3.1
1	B	11	ASP	3.1
1	L	240	TYR	3.1
2	F	212	ASP	3.1
2	H	88	LEU	3.1
2	F	122	ARG	3.1
3	G	647	VAL	3.1
1	A	109	PRO	3.1
1	L	85	ILE	3.1
1	L	161	HIS	3.1
2	F	295	ILE	3.0
1	L	336	LYS	3.0
1	C	274	ILE	3.0
1	A	297	ASN	3.0
1	B	180	LEU	3.0
2	D	250	VAL	3.0
1	C	278	THR	3.0
1	B	32	PRO	3.0
1	M	175	ILE	3.0
3	E	655	ASP	3.0
2	F	192	PRO	3.0
2	H	160	PRO	3.0
1	B	34	ILE	3.0
2	H	283	MET	3.0
1	C	347	ALA	3.0
2	N	170	PHE	3.0
2	H	155	CYS	2.9
2	J	293	PHE	2.9
1	L	83	GLU	2.9
1	L	272	ALA	2.9
1	C	110	LEU	2.9
2	F	88	LEU	2.9
1	A	11	ASP	2.9
2	N	160	PRO	2.9
1	L	169	TYR	2.9
2	N	120	LEU	2.9
1	C	3	ASP	2.9
1	C	108	ALA	2.9
2	H	62	CYS	2.9
2	F	108	LEU	2.9
2	J	294	GLN	2.9
1	A	82	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	336	LYS	2.9
2	H	20	ARG	2.9
2	H	159	LEU	2.9
1	B	309	ILE	2.9
2	N	158	CYS	2.9
2	F	16	LEU	2.9
2	N	121	LEU	2.9
2	J	122	ARG	2.9
2	J	148	LEU	2.9
1	C	162	ASN	2.9
1	L	172	PRO	2.8
3	I	645	GLU	2.8
2	D	204	LEU	2.8
1	A	104	LEU	2.8
1	L	135	ALA	2.8
2	H	190	MET	2.8
3	O	641	VAL	2.8
2	H	182	SER	2.8
2	D	89	PHE	2.8
2	H	161	ILE	2.8
1	C	159	VAL	2.8
1	M	12	ASN	2.8
1	A	86	TRP	2.8
2	D	176	LEU	2.8
2	D	62	CYS	2.8
2	H	16	LEU	2.8
1	B	160	THR	2.8
1	L	75	ILE	2.8
2	N	154	ASP	2.8
2	J	120	LEU	2.8
2	J	33	ASN	2.7
1	C	38	PRO	2.7
2	F	298	PRO	2.7
2	F	204	LEU	2.7
2	H	242	ASP	2.7
1	C	270	GLU	2.7
2	F	121	LEU	2.7
1	M	165	ILE	2.7
1	L	338	SER	2.7
2	F	254	GLY	2.7
1	B	321	ALA	2.7
1	B	58	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	106	THR	2.7
1	M	52	SER	2.7
2	J	281	ALA	2.7
2	H	126	GLU	2.7
1	C	86	TRP	2.7
1	L	160	THR	2.7
2	F	159	LEU	2.7
1	B	274	ILE	2.7
1	C	17	VAL	2.7
2	N	65	ILE	2.7
1	M	161	HIS	2.7
1	C	134	VAL	2.7
1	C	111	ASN	2.7
2	H	300	GLU	2.7
2	J	39	CYS	2.7
1	C	357	ILE	2.7
1	L	105	LEU	2.7
2	F	73	LEU	2.6
1	B	299	MET	2.6
1	B	347	ALA	2.6
1	C	261	LEU	2.6
1	C	369	ILE	2.6
2	J	8	ASN	2.6
1	B	261	LEU	2.6
2	J	25	GLY	2.6
2	N	63	GLY	2.6
2	F	35	ILE	2.6
1	M	25	ASP	2.6
2	F	176	LEU	2.6
2	D	246	ARG	2.6
1	B	196	ARG	2.6
1	L	343	GLY	2.6
2	H	171	CYS	2.6
1	L	162	ASN	2.6
1	A	152	VAL	2.6
1	C	297	ASN	2.6
2	F	59	LEU	2.6
1	B	317	ILE	2.6
1	M	136	ILE	2.6
1	C	9	VAL	2.6
2	J	177	SER	2.6
2	H	19	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	J	162	ALA	2.6
2	H	42	SER	2.6
1	A	63	GLY	2.5
2	J	104	ILE	2.5
1	A	103	THR	2.5
2	H	91	GLY	2.5
1	C	306	TYR	2.5
1	L	2	GLU	2.5
2	D	21	GLY	2.5
2	H	61	ILE	2.5
2	N	104	ILE	2.5
1	B	17	VAL	2.5
1	L	261	LEU	2.5
2	H	40	LEU	2.5
2	N	136	PHE	2.5
3	O	645	GLU	2.5
1	C	89	THR	2.5
2	F	72	LEU	2.5
2	H	107	LEU	2.5
1	B	200	PHE	2.5
2	H	106	LEU	2.5
1	B	278	THR	2.5
1	M	22	ALA	2.5
1	A	83	GLU	2.5
1	M	162	ASN	2.5
1	L	347	ALA	2.5
2	F	102	GLU	2.5
2	D	120	LEU	2.5
2	J	146	ILE	2.5
3	I	655	ASP	2.5
1	L	175	ILE	2.5
2	F	71	ASP	2.5
1	L	346	LEU	2.5
1	L	27	PRO	2.4
2	J	56	GLU	2.4
1	L	3	ASP	2.4
1	B	162	ASN	2.4
2	H	251	VAL	2.4
2	J	30	LEU	2.4
1	A	96	VAL	2.4
2	N	101	LEU	2.4
2	F	51	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	268	SER	2.4
2	F	189	ILE	2.4
1	C	338	SER	2.4
1	A	74	GLY	2.4
2	N	38	LEU	2.4
1	A	347	ALA	2.4
1	C	40	HIS	2.4
2	J	61	ILE	2.4
2	N	127	CYS	2.4
1	A	151	ILE	2.4
1	C	180	LEU	2.4
2	J	89	PHE	2.4
1	A	94	LEU	2.4
2	F	75	LEU	2.4
1	C	102	PRO	2.4
2	F	96	ARG	2.4
1	L	97	ALA	2.4
2	J	266	LEU	2.4
1	A	134	VAL	2.4
1	M	163	VAL	2.4
2	F	55	LEU	2.4
2	N	172	CYS	2.4
2	N	19	VAL	2.4
1	B	336	LYS	2.4
2	J	72	LEU	2.4
1	A	296	ASN	2.4
1	B	59	GLN	2.4
1	L	112	PRO	2.4
2	D	269	ALA	2.4
1	C	107	GLU	2.4
2	J	75	LEU	2.3
2	J	190	MET	2.4
2	D	90	LEU	2.3
1	B	137	GLN	2.3
2	N	252	GLU	2.3
2	D	162	ALA	2.3
2	N	31	GLN	2.3
1	A	293	LEU	2.3
2	J	192	PRO	2.3
1	A	77	THR	2.3
1	L	327	ILE	2.3
1	L	92	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	300	SER	2.3
2	D	107	LEU	2.3
2	F	201	LEU	2.3
1	B	67	LEU	2.3
1	C	94	LEU	2.3
2	J	63	GLY	2.3
2	D	123	GLY	2.3
2	H	65	ILE	2.3
1	B	62	ARG	2.3
1	B	338	SER	2.3
1	B	262	PHE	2.3
1	C	163	VAL	2.3
1	L	5	THR	2.3
1	L	238	LYS	2.3
1	C	63	GLY	2.3
1	L	273	GLY	2.3
2	N	123	GLY	2.3
2	D	105	CYS	2.3
1	L	294	TYR	2.3
1	B	313	MET	2.3
2	D	110	TYR	2.3
2	H	41	LYS	2.3
1	C	133	TYR	2.3
2	N	89	PHE	2.3
2	H	170	PHE	2.3
3	O	647	VAL	2.3
2	F	190	MET	2.3
2	H	210	ASP	2.3
1	A	1	ASP	2.3
1	M	105	LEU	2.3
2	J	159	LEU	2.3
1	A	78	ASN	2.3
1	C	79	TRP	2.3
2	N	36	ARG	2.3
1	L	253	GLU	2.3
1	A	173	HIS	2.2
1	M	149	THR	2.2
1	A	71	ILE	2.2
2	N	93	TYR	2.2
1	M	338	SER	2.2
2	H	183	MET	2.2
2	J	189	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	98	PRO	2.2
1	B	155	SER	2.2
2	H	98	LYS	2.2
1	C	153	LEU	2.2
1	M	174	ALA	2.2
1	B	320	LEU	2.2
1	M	361	GLU	2.2
1	M	86	TRP	2.2
2	D	170	PHE	2.2
2	J	7	LEU	2.2
1	B	249	THR	2.2
1	C	64	ILE	2.2
1	L	331	ALA	2.2
1	M	278	THR	2.2
2	J	283	MET	2.2
2	J	191	ARG	2.2
1	A	298	VAL	2.2
1	A	299	MET	2.2
2	D	183	MET	2.2
2	F	109	ALA	2.2
1	A	9	VAL	2.2
1	C	82	MET	2.2
2	F	82	PRO	2.2
2	F	156	PHE	2.2
1	M	101	HIS	2.2
1	L	133	TYR	2.2
2	F	152	PHE	2.2
2	F	157	ASN	2.2
1	C	170	ALA	2.2
1	A	17	VAL	2.2
1	A	304	THR	2.2
1	C	18	LYS	2.2
2	D	282	MET	2.2
2	F	76	PHE	2.2
2	D	126	GLU	2.2
2	J	37	GLY	2.2
2	H	157	ASN	2.2
1	L	198	TYR	2.1
2	H	43	ARG	2.1
1	L	309	ILE	2.1
2	D	244	ILE	2.1
2	F	170	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	32	GLU	2.1
1	A	138	ALA	2.1
1	C	98	PRO	2.1
1	A	79	TRP	2.1
2	H	293	PHE	2.1
1	L	37	ARG	2.1
3	I	647	VAL	2.1
3	O	643	PHE	2.1
2	D	127	CYS	2.1
2	H	176	LEU	2.1
2	J	9	ILE	2.1
2	N	300	GLU	2.1
2	J	31	GLN	2.1
1	B	322	PRO	2.1
1	C	21	PHE	2.1
1	M	94	LEU	2.1
1	M	363	ASP	2.1
2	H	158	CYS	2.1
1	C	4	GLU	2.1
2	D	195	VAL	2.1
1	C	78	ASN	2.1
1	L	340	TRP	2.1
1	M	154	ASP	2.1
3	I	653	SER	2.1
2	D	300	GLU	2.1
2	F	180	LEU	2.1
1	M	137	GLN	2.1
1	B	282	ILE	2.1
1	M	313	MET	2.1
2	F	253	ASP	2.1
1	L	139	VAL	2.1
2	H	21	GLY	2.1
1	A	337	TYR	2.1
1	B	33	SER	2.1
1	C	282	ILE	2.1
2	N	250	VAL	2.1
1	C	361	GLU	2.1
2	H	143	ARG	2.1
1	C	150	GLY	2.1
1	L	115	ASN	2.1
1	L	237	GLU	2.1
1	M	311	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	30	LEU	2.1
2	F	247	ALA	2.1
2	H	30	LEU	2.1
2	J	144	TYR	2.1
1	L	18	LYS	2.1
3	I	654	GLY	2.1
2	F	101	LEU	2.1
1	B	139	VAL	2.0
2	D	121	LEU	2.0
1	A	200	PHE	2.0
3	I	652	ILE	2.0
1	B	61	LYS	2.0
1	A	323	SER	2.0
1	L	361	GLU	2.0
2	J	296	LEU	2.0
2	H	36	ARG	2.0
1	C	19	ALA	2.0
2	H	169	ILE	2.0
1	L	103	THR	2.0
1	L	278	THR	2.0
2	H	144	TYR	2.0
1	M	366	GLY	2.0
2	N	186	ILE	2.0
1	B	65	LEU	2.0
1	L	20	GLY	2.0
2	J	107	LEU	2.0
2	N	140	CYS	2.0
1	B	177	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

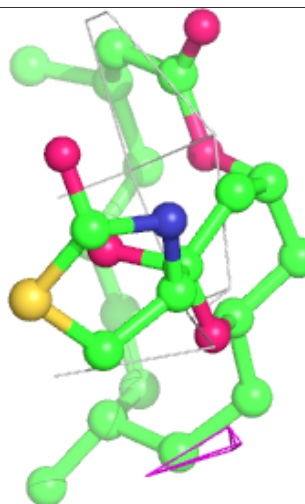
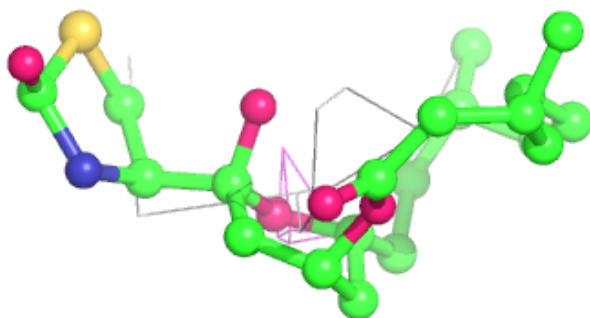
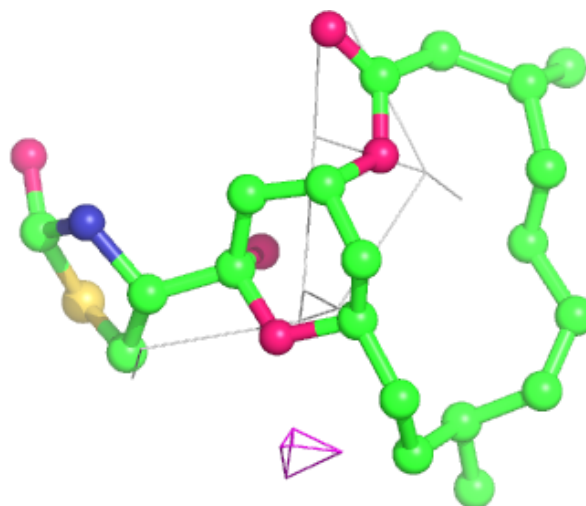
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MN	H	1302	1/1	0.60	0.16	230,230,230,230	0
6	MN	D	1302	1/1	0.66	0.19	165,165,165,165	0
6	MN	J	1302	1/1	0.66	0.17	197,197,197,197	0
6	MN	J	1301	1/1	0.68	0.19	200,200,200,200	0
6	MN	H	1301	1/1	0.69	0.20	234,234,234,234	0
4	LAB	C	1376	27/27	0.69	0.67	253,258,268,271	0
5	ATP	L	1377	31/31	0.71	0.43	290,306,327,332	0
6	MN	F	1302	1/1	0.72	0.24	203,203,203,203	0
6	MN	N	1301	1/1	0.73	0.15	213,213,213,213	0
4	LAB	B	1376	27/27	0.74	0.73	165,173,181,186	0
5	ATP	M	1377	31/31	0.74	0.27	334,341,360,361	0
6	MN	N	1302	1/1	0.75	0.17	213,213,213,213	0
6	MN	D	1301	1/1	0.76	0.27	166,166,166,166	0
6	MN	F	1301	1/1	0.77	0.21	207,207,207,207	0
5	ATP	B	1377	31/31	0.81	0.45	155,160,163,164	0
4	LAB	L	1376	27/27	0.81	0.57	303,322,330,334	0
4	LAB	M	1376	27/27	0.82	0.37	321,332,340,340	0
5	ATP	A	1377	31/31	0.82	0.46	135,137,142,143	0
5	ATP	C	1377	31/31	0.84	0.57	242,246,249,250	0
4	LAB	A	1376	27/27	0.88	0.65	139,142,147,149	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

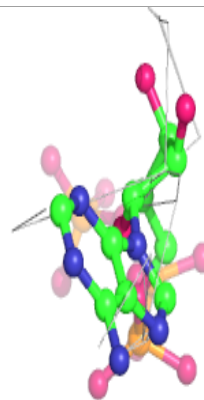
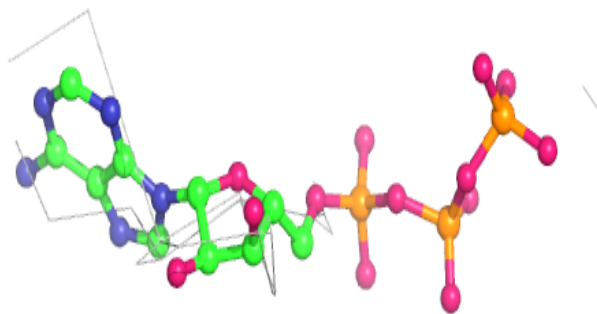
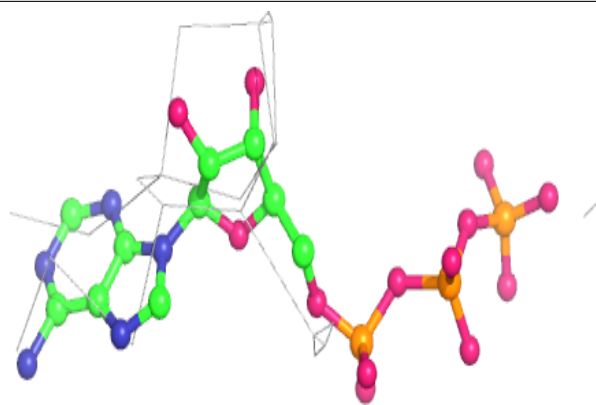
Electron density around LAB C 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



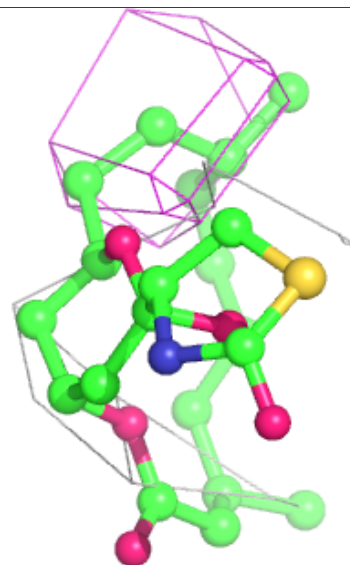
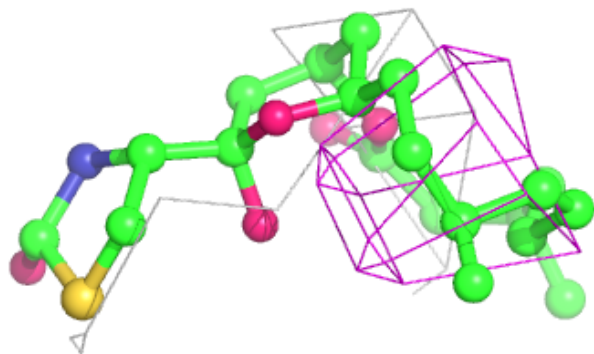
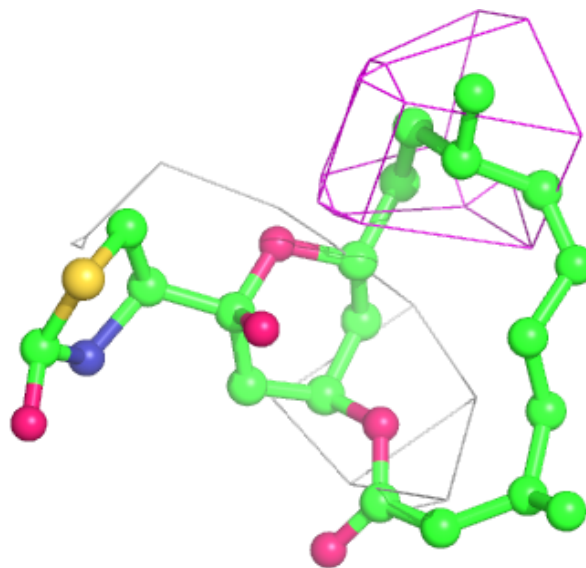
Electron density around ATP L 1377:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



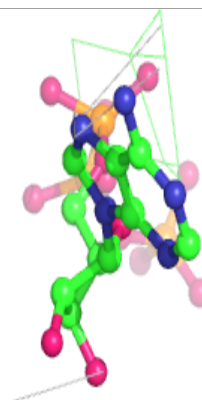
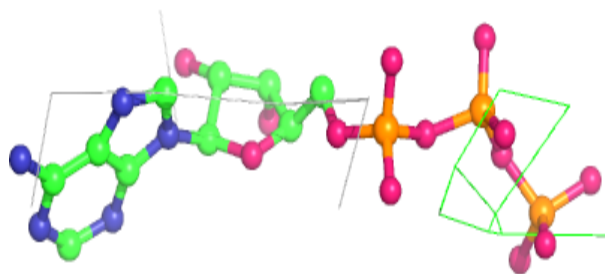
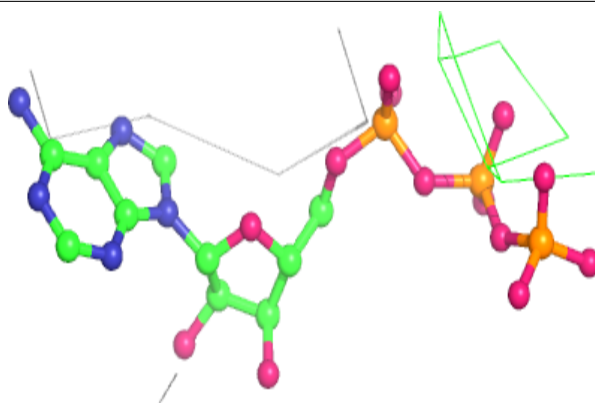
Electron density around LAB B 1376:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

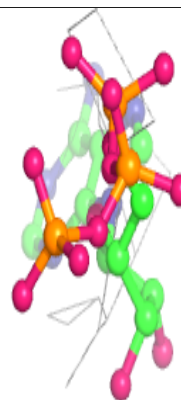
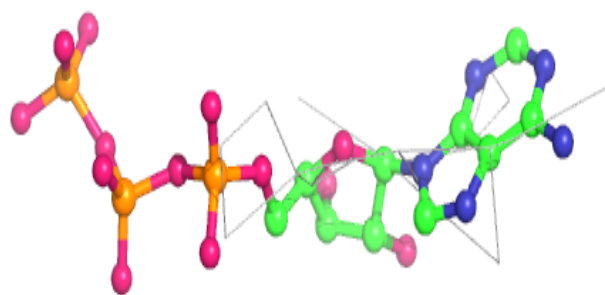
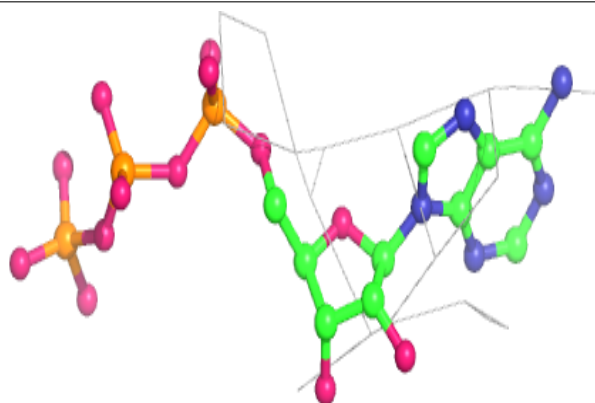


Electron density around ATP M 1377:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

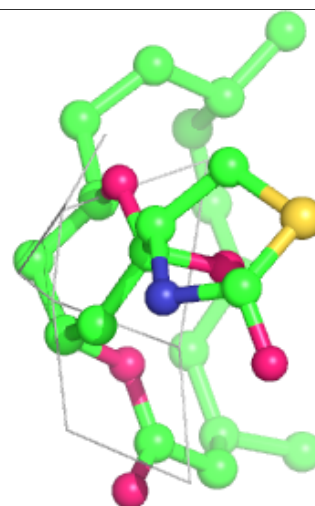
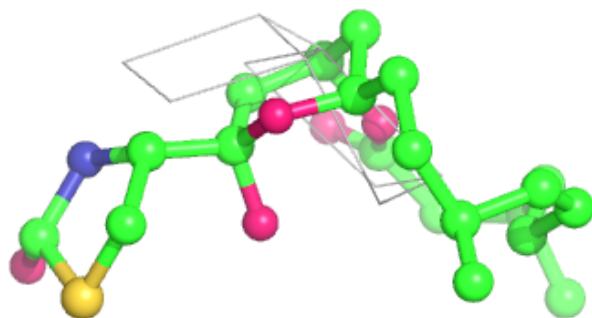
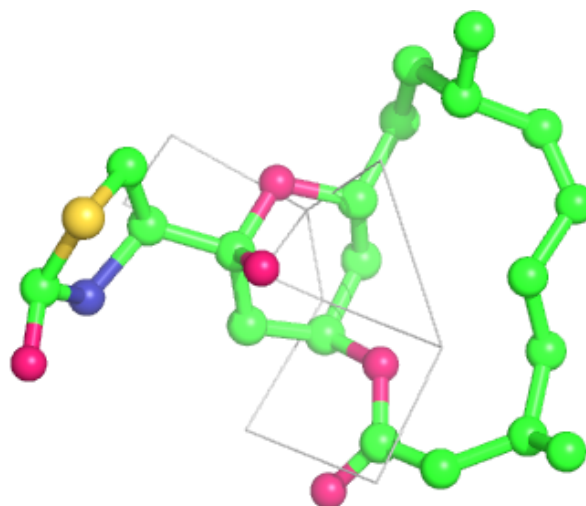
**Electron density around ATP B 1377:**

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



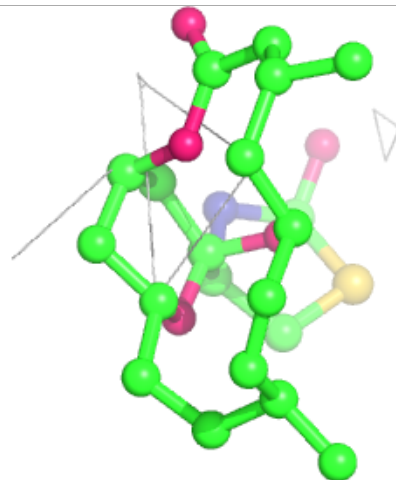
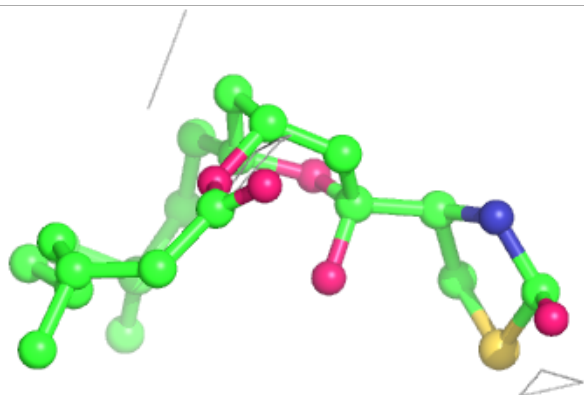
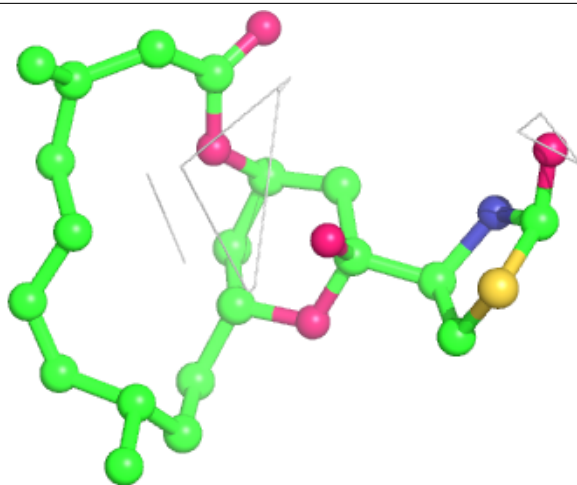
Electron density around LAB L 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



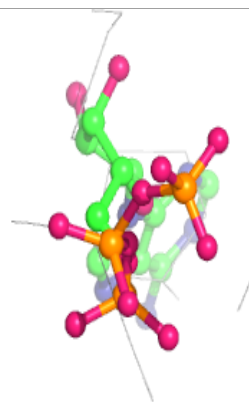
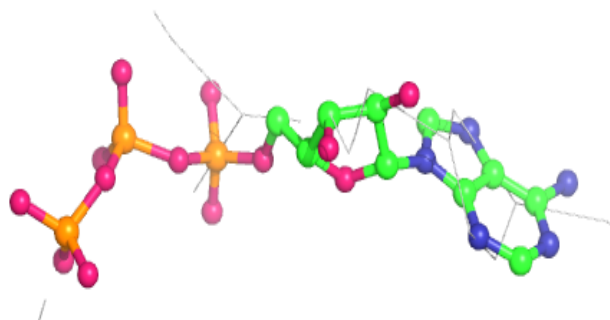
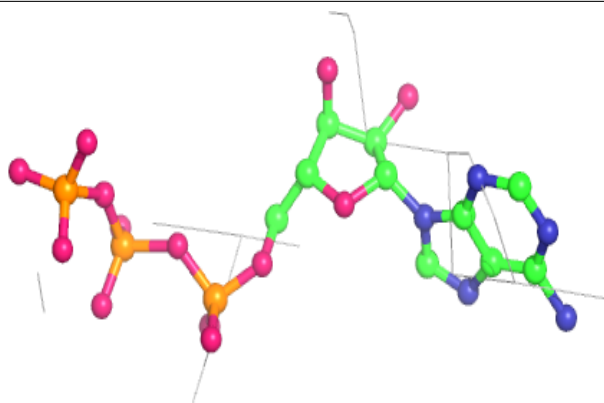
Electron density around LAB M 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

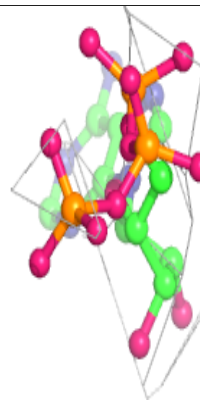
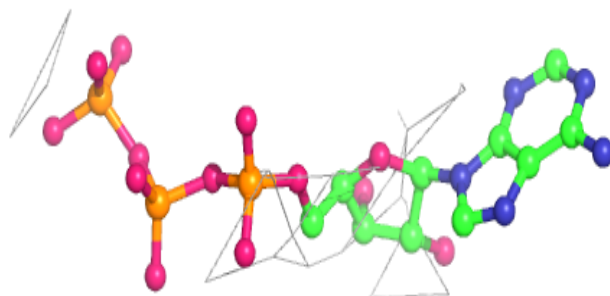
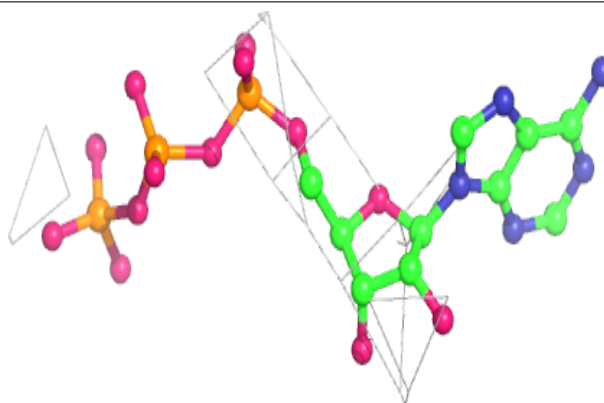


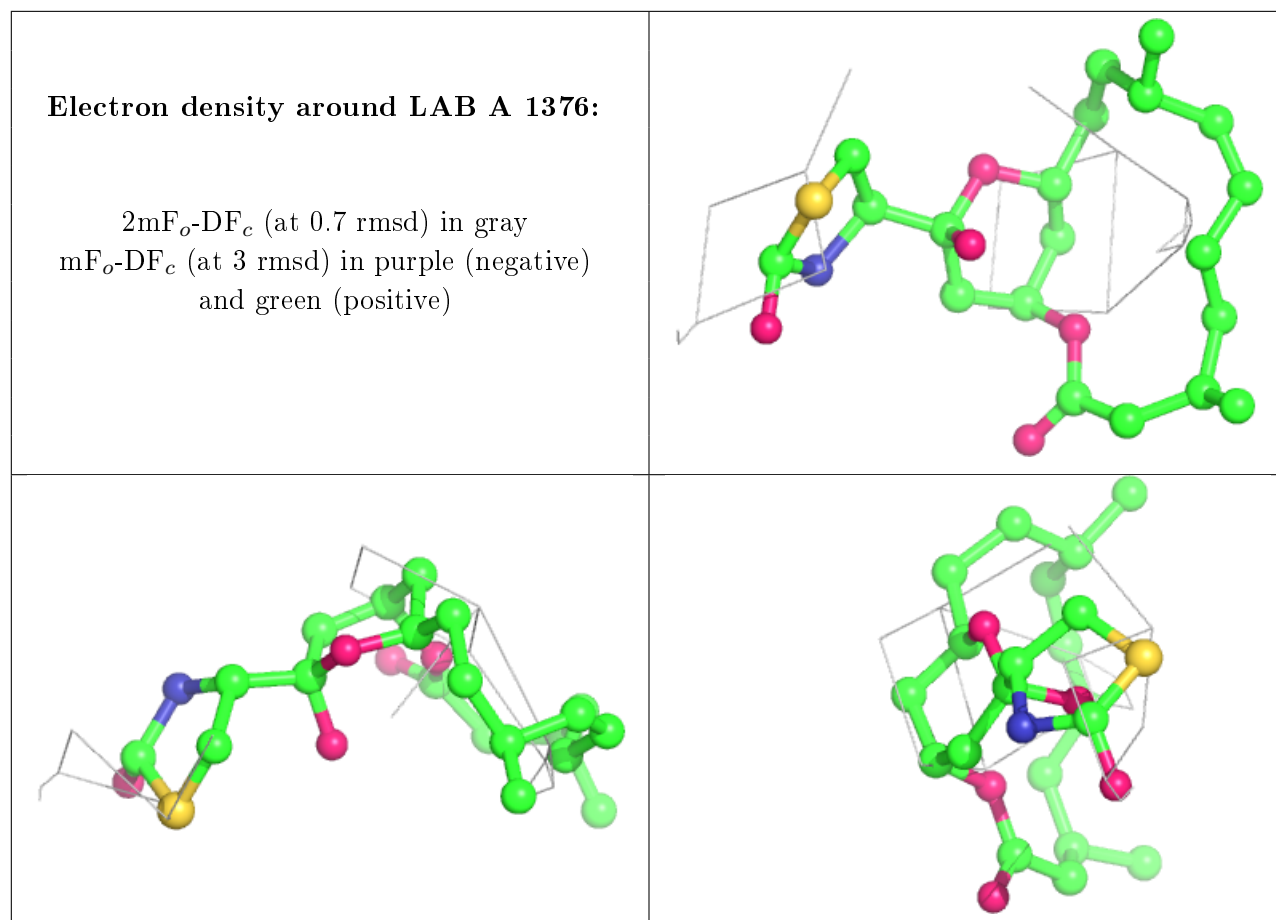
Electron density around ATP A 1377:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP C 1377:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.